Survey on Modeling and Simulation of Multiphysics Systems

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Abstract

This paper presents a retrospective on the evolution of modeling and simulation (M&S) as they relate to multiphysics systems. The context space of M&S is defined in terms of number of fields, number of domains, length scale, and computational technologies involved. Representative past and the present efforts on each one of these contexts and some of their combinations are described and their relationship to the product development efforts of ASME's Computer and Information in Engineering (CIE) division is identified. The general procedures for developing multi-field formulations are given first. Then the multi-domain progress is given with an emphasis on fluid-structure interaction problems pertaining to linear and non-linear aeroelasticity and aerothermoelasticity. Multi-scale methodologies follow, and the computational technologies associated with model generation and simulation is also presented. Potential future anticipated trends and directions are identified and conclude this survey.

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INTRODUCTION

The main goal of the present effort is to present an overview of the past, present and potentially the future evolution in the field of modeling and simulation (M&S) of multiphysics systems from a product development perspective.

On one hand, the extensive pluralism of the ever evolving computational technologies and on the other hand the sharp private focus of individual researchers onto their own subject of interest sometimes prevent an up-to-date comprehensive understanding of how private efforts relate to global history and trends. Thus, besides its ceremonial character relative to honoring the 25th anniversary of the Computer and Information in Engineering (CIE) division of the ASME, the technical component of the motivation for the present work is to provide a reality check reference point for all practitioners of M&S methodologies and technologies as they apply to product development.

Here it should be underlined that while utilitarian and economic pressures push for the development of inexpensive complex products under complex operational conditions, the computational technology evolution provides an ever improving realm of reducing to practice applied science and engineering knowledge. These two factors provide us with the opportunity to anticipate fast, efficient and economically viable development of complex products, the models of which correspond to real-life applications with less simplifications and assumptions than those used in the past.

It is imperative that for the sake of clarity and disambiguation we provide the operational definitions of the fundamental terms associated with our topic.

Today's product development requires the exercise of M&S not only in terms of product appearance and shape but also in terms of the systemic behavior of a product. The first aspect of M&S for shape and appearance deals with what traditionally has been associated with Computer Aided Design (CAD) and and Manufacturing (CAM). However, these are areas explored by another article on the same issue of JCISE []. Our present effort focuses on examining the evolution of M&S in terms of behavioral models for multiphysics systems. In particular, by "modeling" here we imply the activity of forming a mathematical representation (and its algorithmic and computational implementation) of the behavior of the system that captures the relation between input (stimulus) and response (output) state variables or/and parameters characterizing this behavior of the system. By the term "simulation" we imply the computational exercise of the model produced by the "modeling" activity, for the sole purpose of predicting the behavior of the system at hand. Clearly, since this behavior is in many cases given in terms of contour, vector and color intensity artifacts painted on the surface or in the volume of the associated systems, the geometric model of them is implicitly but inextricably associated with the behavioral models.

The usage of the term "multiphysics" has been often used liberally during the past five years by various

researchers. However, it has been used in more than one undeclared contexts not always allowing the occasional consumers of the term to be able to isolate the meaning intended by the originators of the term. Some of the frequently attributed meanings of the term have been those of: "multi-field" to denote the simultaneous excitation and response of the system by multiple physical fields; "multi-domain" to denote the interaction among continuum representations of systems with drastically different properties (e.g. fluid-structure interaction, moving solidification boundary problems e.t.c.) through sharable boundaries; "multi-scale" to denote the consistent bridging of various behavioral models of the system at hand, at various length scales as required by a multitude of scopes ranging from manufacturing process perspective to macro-behavioral utilization. In addition, any combination of these three semantic possibilities generates four more meanings of the term "multiphysics" including the one that reflects the co-existence of all three of them. This suggests the definition of a conceptual attribute space (see Fig. 1) spanned by the three basis attributes namely, "multi-field", "multi-domain" and "multi-scale". All other cases for the potential meaning of the term "multi-field" are embedded implicitly in this space and can be thought of as linear combinations of the three base-cases. In addition, the "multi-field" and "multi-domain" bases are endowed with a measure defined in terms of two discrete increments for "one" and "many". The "multi-scale" base is similarly endowed by a measure defined in terms of the discrete increments in the term set {"nano", "micro", "macro"} roughly corresponding to applying these as prefixes to the term "meter" when used as a length unit.

Any discrete volume in this discrete space as shown in Fig. 1, is defined by a triplet of coordinates originating from each one of these attribute axes, and represents a region encompassing certain classes of physical problems. This signifies that these problems can be modeled in a multiphysics sense as defined by their corresponding coordinates. Our description of the M&S retrospective will be based on references in this space in a manner that corresponds to the authors' individual experiences as they correspond to these base cases of this space.

There are many more attributes of the M&S activities as they relate to the interests of the various stake-holders associated with the production and consumption of M&S methodologies, processes, and products, that can define their own spaces (e.g. implementation technology, manufacturing, business, human factors, technology transfer, direction of modeling, maintainability, software engineering etc.) in a manner similar to the one used above for describing the term "multiphysics". Example base cases for the economical business subspace would be the total cost of ownership, the return on investment and the production cost. Example base cases for the manufacturing subspace would be total production time, yield and efficiency. Examples base cases for the human factors subspace would be confidence measures such as qualification, verification and validation, and usability measures such as slope and length of learning curve etc. However, it falls outside the scope of this paper to address these and the rest of the subspaces mentioned in more detail.

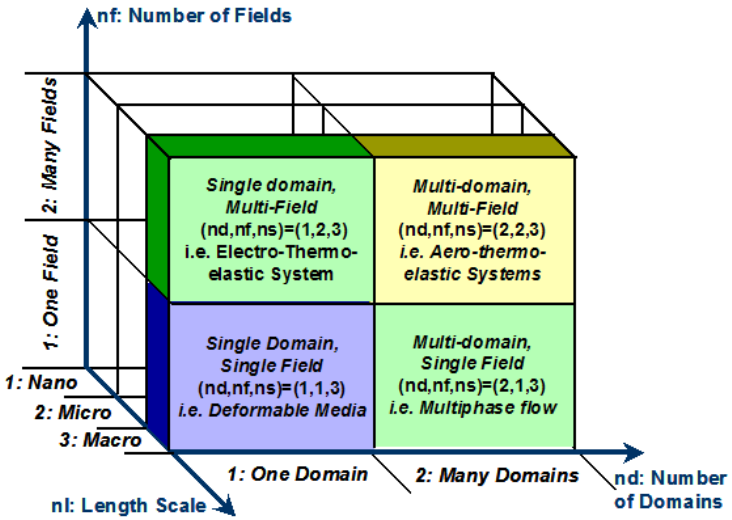

Figure 1: Multiphysics attribute space.

In addition to the three base cases described for the defining the therm "multiphysics", here we will focus only on one of these additional subspaces. This will be the "computational technology implementation" subspace. Activities in this subspace are intimately associated with the progress on M&S as a discipline in its own right because they often provide a motivational pulling mechanism for reducing to practice advances of the associated methodologies and implementations. Space limitations do not allow further decomposition of this attribute space to base cases (e.g. distributed technologies, semantic technologies, data exchange technologies etc.)

Product development efforts based on the research activity efforts on multiphysics systems are far less compared to the "single" physics system modeling, mainly due to the inherent complexity associated with them. Therefore, this paper will be focusing less on the history and more on the available methodologies and technologies as opportunities for future product development via the catalytic leveraging of the independent progress of the computational technologies.

Therefore, this paper contains descriptions of the evolution of M&S in terms of the four base cases of multi-field, multi-domain, multi-scale formulations and computational technologies. We initially define the abstract formulation context for these cases in order to facilitate the development of their retrospective views. Our survey will address all four of them in separate sections and will cover the past and the present state of affairs. The speculated future evolution of these areas will be discussed in the next section. The paper will close with appropriate conclusions.

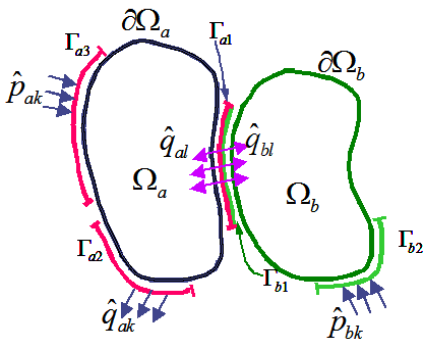

Figure 2: Interacting multi-domain and multi-filed continuum systems idealization.

MULTI-FIELD MULTI-DOMAIN FORMULATION CONTEXT

Figure 2 depicts two (out of possibly many) interacting continua under the influence of multiple fields. We are using this figure to present a general formulation of a mathematical model describing the behavior of multiple interacting continua under multi-field conditions at a given length scale as the following system of generally coupled equations,

$$\mathcal{D}_{di}(\hat{q}_{dj}, \hat{p}_{dj}; \dot{\hat{q}}_{dj}, \dot{\hat{p}}_{dj}) = 0, \text{ on } \Omega_d \tag{1}$$

. Here the indices are defined by, $i \in [1, ne]$, $j \in [1, nf]$ and $d \in \{a, b, \ldots, nd\}$, where ne, nf and nd are the number of equations, the number of conjugate field pairs and the number of domains respectively. The operator $\mathcal{D}_{di}$ (usually differential) expresses some conservation law and is defined per equation per domain while it represents the nature of the behavior of the system as defined by conjugate state variable pairs $< \hat{p}_{dj}, \hat{q}_{dj} >$ and for some cases their time derivatives $< \dot{\hat{p}}_{dj}, \dot{\hat{q}}_{dj} >$. Algebraic closure of Eqs. In most cases in the bibliography, the quantities $\hat{p}_{dj}$ and $\hat{q}_{dj}$ reflect the dependent and independent variables of the formulation, or the input-output variables of the system. They can be components of tensor variables of any order, but usually are scalars, vector components, or second order tensor components. This intention is represented by the hat-bold notation used.

To fully determine the $2 \times nf$ field variables, algebraic closure of the system of Eqs. (1) requires that $ne \geq 2\times$. The factor 2 appears because the field variables and their derivatives occur in conjugate pairs (e.g. $< stress, strain >, < temperature, entropy >$, etc.) Since the number of conservation laws that end up providing (in most cases) these equations is small and independent of the particular problem, it is evident that additional relations between the state variables are needed. This is where the constitutive field theory (CFT) generation process has to be invoked in terms of the determination of constitutive $nd \times nf$ functionals $\mathfrak{C}_{dj}$ that usually relate the first member of the conjugate state variable pair with the second one according

to,

$$\hat{q}_{dj} = \mathfrak{C}_{dj}(\hat{p}_{dj}; \dot{\hat{p}}_{dj}), \text{ in } \Omega_d \tag{2}$$

.

After proper term elimination and rewriting this equation reduces the field Eqs. (1) in the form,

$$\mathcal{D}_{di}(\hat{q}_{dj}; \dot{\hat{q}}_{dj}) = 0, \text{ in } \Omega_d. \tag{3}$$

Algebraic closure of this system requires that $ne \geq nf$. Sometimes, either because the corresponding CFT does not succeed in algebraically completing the set of Eqs. (1) by providing an adequate number of equations, or because special formalistic restrictions are required (i.e. fading material memory, frame reference invariance etc.), additional axioms may be introduced. The term reduction/rewriting procedure mentioned earlier, always requires that the system of Eqs. (1) and (2) is equivalent with the system of Eqs. (3).

Either of these formulations is typically equipped with their corresponding Dirichlet and Neumann boundary conditions applicable on both the interacting (shared) manifolds $\Gamma_{a1} = \Gamma_{b1} \subset \partial\Omega_a \cap \partial\Omega_b$ of the domains, and the non-interacting ones $\Gamma_{ab} \subset \partial\Omega_a - \partial\Omega_a \cap \partial\Omega_b$ and $\Gamma_{bb} \subset \partial\Omega_b - \partial\Omega_a \cap \partial\Omega_b$, where the second subscript of all Γs is defined by $b \in [1, nnsbd]$ where $nnsbd$ is the number of non shared boundary domains. Typically, fields present to both domains express boundary conditions over the sharable interacting boundary manifold in the form of transmission conditions preserving conservation principles and they are usually of the type,

$$\hat{p}_{ai} \cdot \boldsymbol{n} = \hat{p}_{bi} \cdot \boldsymbol{n} + \mathfrak{T} \text{ on } \Gamma_{a1} = \Gamma_{b1} \tag{4a}$$

$$\dot{\hat{p}}_{a(i+1)} = \dot{\hat{p}}_{b(i+1)} \text{ on } \Gamma_{a1} = \Gamma_{b1}. \tag{4b}$$

Here, $\boldsymbol{n}$ denotes the unit normal vector on $\Gamma_{a1} = \Gamma_{b1}$, and $\boldsymbol{\mathfrak{T}}$ the disturbance vector normal to $\Gamma_{a1} = \Gamma_{b1}$ that may appear due to not interaction related reasons.

Most multi-field and multi-domain applications involving interacting systems that can be represented as deformable continua with shared boundary manifolds can be captured from the above presented set of generalized equations.

MULTI-FIELD RETROSPECTIVE

There is a plethora of contemporary devices that are used as sensors and actuators. It is often forgotten that these devices along with their associated application methodologies always exploit some form of field coupling. Typical examples are displacement and/or strain sensors and actuators that use electro-elastic

coupling. However, this is almost always done in the context of very simple (mostly one-dimensional) systems with only single field coupling capability (i.e. strain gauges, piezo-electric load cells etc.) On the other hand, today's demands for complex multifunctional systems in combination of continuously tightening economical requirements beg for a drastic reconsideration of product development practices. For example, establishing design allowables on an complex engineering structure that is exposed to mechanical, thermal and humidity stimulus, like the composite material skin of an aircraft, by only considering the influence of each of the stimuli separately and subsequently superimposing the design recommendations produced by each one of the modeling practices for each one of these stimuli, almost always results to over-designed and non optimized systems. It is therefore imperative to re-examine the often forgotten assumptions of non interacting fields on the structure and consider the employment of coupled-field M&S practices and methodologies.

The evolution of multi-field modeling of deformable media has seen a variety of approaches that were motivated by a wide range of interests, and were based on a wide range of backgrounds and techniques. Multi-field modeling problems are represented by area (1,2,3) when only one one domain is involved (single system) in the context space presented by Fig. 1.

The first coupled-field phenomena had been experimentally observed for thermoelectricity by Seebeck on 1821 (Seebeck Effect) and Peltier on 1834 (Peltier Effect) [1]. Soon after this, Duhamel gave the first multi-field (though uncoupled) formulation for the case of thermoelasticity and postulated the coupled case [2].

The first fully developed multi-field formulation for a deformable medium was given by Navier who gave the well known Navier-Stokes equations for an incompressible fluid in 1821 [3] and a viscous fluid in 1822 [4]. Maxwell in his classical and foundational work on electrodynamics [5, 6] gave the second fully developed multi-field formulation. This formulation did not address the idea of a "deformable" continuum explicitly, but it was formulated upon the assumption that a continuum called "aether" occupied the space between conductors and insulators. This work though by contemporary standards constitutes the basis of the fundamental theory of electrodynamics of continua, it was originally viewed and evolved as a theory for electromagnetics for its applicability to wave propagation and field force applications.

The first truly coupled multi-field formulation for deformable solids contains the heat conduction equation endowed with strain terms and was given by Voigt [7] and Jeffreys [8] and thermal stresses solution were given by Papkowitch [9] and Sokolnikoff [10]. However the real development of coupled thermoelasticity started with Biot [11]. This effort has been based on irreversible thermodynamics as it was founded a few years earlier by Onsanger [12, 13] and popularized by Prigogine [14] and de Groot [15] who were able ro show that non-equilibrium thermodynamics are needed to capture the irreversible character of heat and mass

diffusion. Their work represents the first systematic efforts for coupled multi-field formulation and it was motivated from chemically reacting species diffusion combined with heat conduction in a continuum system. After this foundational work, the actual area of multi-field modeling for deformable continuum systems has evolved starting mainly from the mid-1950s, with short periods of intensification. It was mostly motivated from the need to develop complete and thorough constitutive models for various material systems at the continuum level with no particular application in mind for most of these attempts. The field has evolved with the development and maturation of two-field modeling theories such as those of thermoelasticity [16, 17, 18], electroelasticity [19, 20], piezoelasticity [21] and magnetoelasticity [22]. It continued with the three-field theories of magnetothermoelasticity [23, 24], thermoelectroelasticity [25], hygrothermoelasticity [26], the four-field theory electromagnetic thermoelasticity [27] and finally, the five-field theory of electromagnetic hygrothermoelasticity [28]. Here we have only cited representative works that are not meant to be inclusive of all work done on the field but they contain more extensive citations on the corresponding theories.

The entire body of work on the multi-field formulation can be classified to belong to one of seven distinct classic approaches. Here we are presenting the three more popular and dominant ones. Their classification is based on the fundamental assumptions employed.

The first group of works is based on assuming that (i) the conservation laws of mass, momentum, moment of momentum, and energy, are holding, (ii) that there exists a thermodynamic potential function that implicitly encapsulates all constitutive equations defining all state field variables, (iii) that entropy as the conjugate scalar field variable of temperature, is governed by an entropy balance law (expressed as a continuity equation) that contains positive definite entropy production, and (iv) that there exist phenomenological forces and fluxes responsible for the irreversible processes involved that obey Onnsager's relations. Extensive exposition of this approach has been given in the 60s [29, 30] and republished later [31, 32].

The second group of works is based on assumptions (i) and (ii) as above but it does not require assumptions (iii) and (iv), while the role of the second law of thermodynamics is played by the Clausius-Duhem inequality [33, 34, 35] (v). The most rigorous, elegant and axiomatically founded formulation of this approach is exemplified by the work of Eringen and his co-workers [27] on electrodynamics of continua. This approach also systematized the usage of the so-called axioms of constitutive theory. These are the axioms of "causality", "determinism", "equipresence", "objectivity", "material invariance", "neighborhood", "fading memory", and "admissibility". The admissibility axiom postulates that the CFT has to satisfy the conservation laws and therefore, it really a meta-axiom in that allows the researcher to postulate the rest of the axioms.

The third group of works comes from the school that attempted and succeeded in axiomatically and very elegantly formalizing all field theories of continua. This approach still uses assumptions (i) and (v), but does

not require assumptions (ii) (though this assumption was introduced later for the special case of Elasticity and Hyperelasticity), (iii) and (iv). While at NRL (1948-51) Truesdell and Toupin solidified this approach that first appeared on 1952 [36] and then it was expanded and presented in the foundational work of "The Classical Field Theories" in 1960 [37]. After the seminal work of Coleman and Noll [38, 39, 40] who used the entropy inequality to construct a unified theory for thermoelasticity and material thermodynamics in general, Truesdell and Noll extended material field theories in the non-linear regime with the equally foundational work of "Non-Linear Field Theories of Mechanics" [41]. It is important to underline here the fact that this work begins with the construction of constitutive relation functionals independent of any thermodynamic potential. However, later the internal strain energy density is used for recovering the constitutive equations, thus reintroducing assumption (ii).

Finally, the fourth group of works is based only on the energy conservation principle (i.e. partial usage of i) while the rest of the conservation laws including conservation of local entropy are all derivable from the energy conservation principle. This is the most recent approach and was formulated by Green and Naghdi [42, 43, 44]. In our view this approach entails the elegance of the fewest possible assumptions and axioms.

An example of following the practices from the first and second groups was recently given for the case of 2-species-hygro-electro-thermo-elastic modeling of ionic polymer-metal composites (IPMC) used for artificial muscle applications. This system's behavior is described by 32 field variables (16 conjugate pairs) governed by 16 field PDEs and 16 equations for the CFT. Introducing equilibrium conditions for many of these fields and Lagrange strains to account for large deformations the case of an electro-elastic isotropic plate becomes a non-linear system of the generalized Von-Karman equations [45, 46]:

$$\nabla^2\nabla^2 w + (1+\nu)\nabla^2 V = \frac{h}{N}(\frac{q}{h} + F_{,22}w_{,11} - 2F_{,12}w_{,12} + F_{,11}w_{,22}), \tag{5a}$$

$$\nabla^2\nabla^2 F + E\nabla^2 V = E[(w_{,12})^2 - w_{,11}w_{,22}], \tag{5b}$$

$$\frac{1-\nu}{2E}(\nabla^2\delta_{ij} - \partial_i\partial_j)F\delta_{ij} + \nabla^2 V = 0. \tag{5c}$$

Here w, F, V are the deflection, the Airy stress function and the electric potential variables and $\delta_{ij}, \nu, E, h, N, q$ are Kronecker's delta, Poisson's ratio, the modulus of elasticity, the plate thickness, the flexural rigidity and the distributed load respectively.

In terms of ASME's CIE division activities in this area only recently there were presentations of work in the context of electroactive ionic polymers behavior motivated by artificial muscle system design [45], as well as fire simulation driven reactive flow [47]. It is forceable that efforts in this area have not been presented in the CIE fora as much, because traditionally CFT modeling has been associated with the activities and fora of the Applied Mechanics division.

MULTI-DOMAIN RETROSPECTIVE

There is a large variety of applications that fall in the category of multi-domain problems. These include multi-phase flaw (e.g. fluidized beds, geomechanics, etc.), phase transformation (e.g. solidification, welding, dendritic growth, material processing etc.), and moving boundaries problems (e.g metal forming, crystal growth, Hele-Shaw flow, Stokes flow, fluid-structure interaction etc.). To report on the evolution of all of these application areas falls well outside the scope and the space available for this paper. Four reasons justify our decision to focus on the fluid-structure interaction problem in the present paper. The first one is its significant importance to product development for a wide variety of applications extending from the design of naval and aero-space structures, to reactive flow induced structural degradation applications. The second one is the fact that its mathematical formulation represents arguably a large subset of moving boundary problems. The third one is that it lends itself to become a vehicle of demonstrating its potential to capture not only the multi-domain aspects of multiphysics modeling but the multi-field one as well. The fourth and final reason stems from the fact that it provides an opportunity to demonstrate that for multi-domain modeling sometimes capturing the physics of the interacting domains may not be enough, and special fields have to be introduced for artificial field-entities applied to discretization-induced entities (i.e. mesh of the fluid domain surrounding the structural domain), in order to preserve the validity of various conservation laws that enforce appropriate field transmission conditions across common boundaries.

Multi-domain modeling problems are represented by area (1,2,3) when only one one field is involved (single physics) in the context space presented by Fig. 1.

Motivation for the Two-domain Multiphysics of Aeroelasticity

A large amount of work on the area of multi-domain multiphysics modeling with moving boundaries has its roots to Aeroelasticity. Aeroelasticity is the theory that models the effects of aerodynamically induced forces on elastic bodies. These effects occasionally lead to serious consequences on the general structural response and stability characteristics for both static and dynamic cases. Consequently, these effects may have a great impact on performance and safety issues, and they have led aeroelasticity to become one of the most important considerations in aircraft design.

Historical literature on aeroelasticity is mostly focused to analytical models where the motion of a gas or a fluid past a structure, the deformation and vibration of that structure, and more importantly, the fluid-structure interaction phenomenon itself, are described with linear mathematical concepts [48, 49]. In the aerospace industry, aeroelastic phenomena are often predicted by linear numerical models and methods that operate in the frequency domain [50, 51]. These methods proloferated quickly because of their high performance and low memory requirements. In the subsonic regime, most if not all of these linear aeroe-

lastic tools rely on the doublet-lattice method [52] for predicting the unsteady aerodynamics of an aircraft. This method was developed over thirty years ago, and remains today the most frequently used method for predicting behavior of unsteady subsonic flows in production environments, especially for analysis involving load and flutter. Furthermore, in the supersonic regime, various linear methods related to the old piston theory [53], are still used today for the prediction of the unsteady aerodynamics acting on an aircraft. For these and various other reasons [54], it can be concluded that no major developments in computational aeroelasticity have occurred since the advent of the piston theory and doublet-lattice methods, and no new major advancements are needed or can be expected.

However, today's high-performance military aircraft while at high dynamic pressure, are often flutter-critical in the transonic speed range. The associated mixed subsonic-supersonic flow patterns and shock waves in this regime lender invalid the linear flow theory in general – and the doublet-lattice method in particular –. They cannot predict the unsteady aerodynamic forces acting on an aircraft. As a result, flutter testing of a scaled model in a transonic wind tunnel has always been used to generate corrections to flutter speeds computed by linear methods. The design, construction, and testing of a wind tunnel flutter model, and the analysis of the resulting data, are very laborious and typically require over a year's time. This explains why recently domain experts have suggested that the results of a finite number of (nonlinear) Computational Fluid Dynamics (CFD) solutions could be used as a surrogate to wind tunnel testing, provided a validated code would be available. Experience had proven that existing CFD codes should be able to compute five flutter solutions in one year [55].

Furthermore, modern military aircraft equipped with external storage tanks and/or weapons are in a flow regime leading to shock waves and on onset of separation, they exhibit Limit Cycle Oscillations (LCO) at transonic Mach numbers. LCO is a nonlinear aeroelastic behavior characterized by periodic oscillations that maintain constant amplitude over time for a given set of flight conditions. Hence, whereas flutter can be catastrophic and must be avoided at all costs, LCO is essentially inducing an accumulation of degradation (e.g. it induces fatigue for metal aircraft components and damage for composite aircraft components) that can have far reaching material degradation consequences leading to acceleration of aging. Linear flutter analysis appears to adequately identify the oscillation frequency and modal composition of the LCO mechanism. However, it predicts unbounded oscillations whereas flight-tests reveal limited amplitude oscillations. More importantly, linear aeroelastic tools fail to predict the onset and severity of LCO which are of prime importance in the certification of external storage tanks and weapon configurations on fighter aircraft [56].

In addition, linear aeroelastic tools are not reliable for high-angle of attack flight conditions. These conditions are sometimes encountered during maneuvering and the flow can separate while its fluctuations

can cause severe buffeting.

Eventually, nonlinear aeroelastic computational fluid dynamics (CFD) tools emerged two decades ago to address local transonic effects, LCO, high-angle of attack flight conditions, buffeting, as well as many other nonlinear aeroelasticity phenomena [57] that cannot be predicted reliably by linear aeroelastic numerical methods. Initially, attention was focused almost exclusively on computational algorithms for transonic unsteady aerodynamics, and applications to simplified linear structures [58]. Subsequently, the scope of nonlinear computational aeroelasticity expanded to address the coupling of individual fluid and structural analysis codes [59], and the exchange of aerodynamic and elastodynamic data between such codes [60]. The recent advances in computational sciences and parallel processing have contributed towards the emergence of complete and real aircraft configurations [61, 62, 63, 63, 64, 56].

In order to provide a description of the current status of approaches for designing and assembling a general purpose nonlinear aeroelastic computational simulation technology, we provide the overview of a particular approach. This approach is based on the three-field, two-domain mathematical formulation of aeroelastic problems and was introduced ten years ago [65]. This three-field formulation exhibits versatility as it can address many aeroelastic problems besides flutter, LCO, and buffeting. These include, the prediction of steady and unsteady loads, the evaluation of control surface effects in level-flight and during maneuvering [66], the prediction of roll damping, aeroelastic tailoring [67, 68], and performance analysis. In this nonlinear aeroelastic formulation and associated computational technology, the aerodynamic forces acting on an aircraft are determined from the solution of the compressible Euler or Navier-Stokes equations with turbulence modeling. Important benefits of this approach are that the aircraft motion is not restricted to harmonic vibrations with small displacement amplitudes, and is not necessarily represented by a truncated modal basis. When appropriate, nonlinear geometric and free-play effects are properly accounted for. Furthermore, no restriction is imposed on the nature of the fluid-structure coupling that is numerically modeled by suitable fluid-structure transmission conditions.

The Three-Field, Two-Domains Formulation of Aeroelastic Models

Motion of some of the fluid domain boundaries is a common characteristic of a large variety of nonlinear fluid-structure interaction problems that are of concern to aerospace, mechanical, civil, and biomedical engineering (i.e. aircraft flutter, flow-induced pipe vibrations, stability of suspension bridges, atrial flutter). The effect of small amplitude motion on the solution of the problem can be handled by simple transpiration techniques [69]. On he other hand, when the amplitude is large, it may become necessary to explicitly address the motion of at least the fluid-structure interface, by a "level set" method [70], or solve the fluid equations on a moving and possibly deforming grid. Such a grid is often referred to as a dynamic mesh in

the computational aerodynamics literature. Many techniques have been developed for solving fluid-structure interaction problems on dynamic meshes, including the Arbitrary Lagrangian-Eulerian (ALE) method [71], the co-rotational approach [72, 73], and space-time formulations [74, 75]. Generally , all of these methods can be used to express the fluid-structure problem of interest as a two domain and three- rather than two-field problem [65].

In fact, if we let $\tilde{\boldsymbol{\chi}}_t$ denote a continuous mapping from a reference fluid configuration $\Omega_F(t)|_{t=0} \subset \mathbb{R}^3$ to a current fluid configuration $\Omega_F(t) \subset \mathbb{R}^3$ such that

$$\boldsymbol{\chi}_t : \Omega_F(t)|_{t=0} \longrightarrow \Omega_F(t), \boldsymbol{x}(\boldsymbol{\xi}, t) = \boldsymbol{\chi}_t(\boldsymbol{\xi}), \tag{6}$$

where $t \in [0, \infty]$ denotes time, $\boldsymbol{x}(\boldsymbol{\xi}, t)$ denotes time-dependent position vector of a fluid point, and $\boldsymbol{\xi}$ its position in reference configuration, while $J = |\partial \boldsymbol{x}/\partial \boldsymbol{\xi}|$ denotes the Jacobian determinant of the deformation gradient, then the system of Eqs. (1) for this case takes the specific form,

$$\left.\frac{\partial (J\boldsymbol{w})}{\partial t}\right|_{\boldsymbol{\xi}} + J\boldsymbol{\nabla}_{\boldsymbol{x}} \cdot (\boldsymbol{F}(\boldsymbol{w}) - \left.\frac{\partial \boldsymbol{x}}{\partial t}\right|_{\xi} \boldsymbol{w}) = J\boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \boldsymbol{R}(\boldsymbol{w}) + J\boldsymbol{S}(\boldsymbol{w}), \text{ in } \Omega_F \tag{7a}$$

$$\rho_S \frac{\partial^2 \boldsymbol{u}_S}{\partial t^2} - \boldsymbol{\nabla}_{\boldsymbol{x}} \tilde{\boldsymbol{\sigma}}_S(\tilde{\boldsymbol{\epsilon}}_S) = \boldsymbol{b}, \text{ in } \Omega_S \tag{7b}$$

$$\rho_f \left.\frac{\partial^2 \boldsymbol{x}}{\partial t^2}\right|_{\boldsymbol{\xi}} - \boldsymbol{\nabla}_{\boldsymbol{\xi}} \tilde{\boldsymbol{\sigma}}_f(\boldsymbol{x} - \boldsymbol{x}|_{t=0}) = 0, \text{ in } \Omega_F \tag{7c}$$

Equation (7a) represents the ALE form of the Navier-Stokes equations where $\boldsymbol{w}$ denotes the conservative fluid state vector, $\boldsymbol{F}$ and $\boldsymbol{R}$ denote the vectors of convective and diffusive fluxes respectively and $\boldsymbol{S}(\boldsymbol{w})$ denotes the source term associated with a potential turbulence model. Equation (7b) is the equation governing the dynamics of the structure represented by its domain $\Omega_S(t) \subset \mathbb{R}^3$. In this equation ρ_S, $\tilde{\boldsymbol{\sigma}}_S$, $\tilde{\boldsymbol{\epsilon}}_S$, $\boldsymbol{u}_S$ and $\boldsymbol{b}$ are the density, the second order stress and strain tensors, and the displacement and body forces vectors respectively. Relationship $\tilde{\boldsymbol{\sigma}}_S(\tilde{\boldsymbol{\epsilon}}_S)$ represents the constitutive functional introduced by the general case earlier through Eq. (2) for the conjugate pair $< \tilde{\boldsymbol{\sigma}}_S, \tilde{\boldsymbol{\epsilon}}_S >$. When it is linear, then it is known as Hooke's constitutive law, and the set of Eqs. (7) represent aeroelasticity. If it is not linear then the set of these equations represent a more general case that allows accounting for degrading materials to the extend that the CFT formulation captures the nonlinearities of such phenomena.

The third of the above equations does not have direct physical origins since it models the dynamics of the fluid mesh motion by assimilating it with a fictitious or pseudo-structural subsystem. The fluid mesh is an artifact of the discretization needed for the integrating the fluid state vector equation and therefore is not a physical quantity. However, the heterogeneous nature and origins of the meshes used for the structure

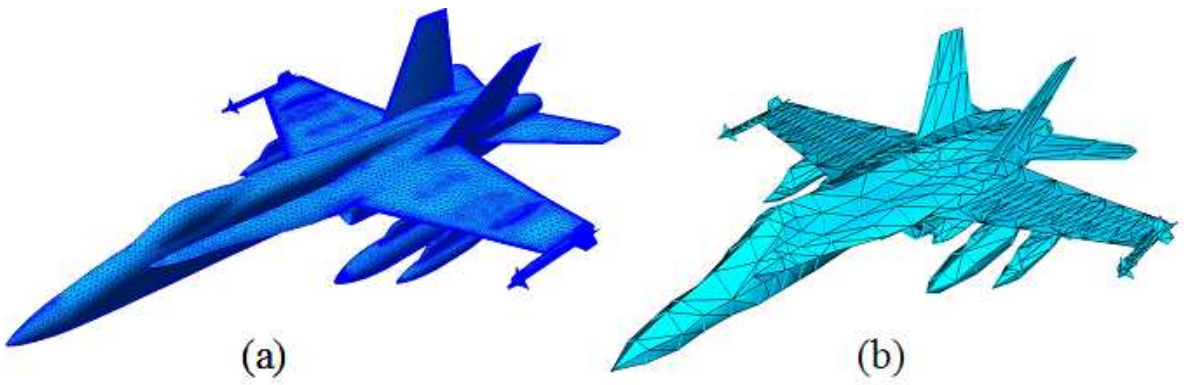

Figure 3: Fluid (a) and structural meshes of the wet surface od an F/A-18 model.

and the fluid (see Fig. 3), introduces the issue of maintaining kinematic compatibility between them while at the same time the conservation laws are not violated. These requirements are indirectly inducing physical meaning of a deformable body on the fluid mesh in a manner that completes the system of equations. An alternative interpretation of this equation is that of a governing equation of a fictions field acting on the fluid. In this last equation, subscript f designates the fictitious nature of the continuous subsystem and its properties, and the initial position of the dynamic fluid-mesh, $\boldsymbol{x}(0)$, is given, while the field to be determined is the current position $\boldsymbol{x}(t)$ of the fluid-mesh. Tilded symbols denote second order tensor field state variables.

The above equations are completed with their Dirichlet and Neumann boundary conditions, that are coupled at the moving fluid-structure boundary $\Gamma(t) = \partial\Omega_F \cap \partial\Omega_S$ by the conditions

$$\tilde{\boldsymbol{\sigma}}_S \cdot \boldsymbol{n} = (-p + \tilde{\boldsymbol{\sigma}}_F) \cdot \boldsymbol{n} + \boldsymbol{\mathfrak{T}}), \text{ on } \Gamma(t), \tag{8a}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{v}, \text{ on } \Gamma(t), \tag{8b}$$

where $\boldsymbol{n}$ denotes the unit normal to $\Gamma(t)$, p the fluid pressure, $\tilde{\boldsymbol{\sigma}}_F$) the viscous (deviatoric) stress tensor of the fluid, $\boldsymbol{v}$ the fluid velocity vector field, and $\boldsymbol{\mathfrak{T}}$ the tractions due to external forces of non aerodynamic origin. For invicid flows these equations have a slightly different form [56]. In addition, the following compatibility conditions hold:

$$\boldsymbol{x}(t) - \boldsymbol{x}(t)|_{t=0} = \boldsymbol{u}, \text{ on } \Gamma(t), \tag{9a}$$

$$\frac{\partial \boldsymbol{x}}{\partial t} = \frac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{v}, \text{ on } \Gamma(t), \tag{9b}$$

The three-field formulation has shed new light on the mathematical understanding of the numerical behavior of various numerical methods that were designed for the solution of coupled fluid-structure problems, and has enabled the development of faster aeroelastic solution algorithms. It led into the development of space and time integration techniques that can exploit efficiently various parallel computational infrastruc-

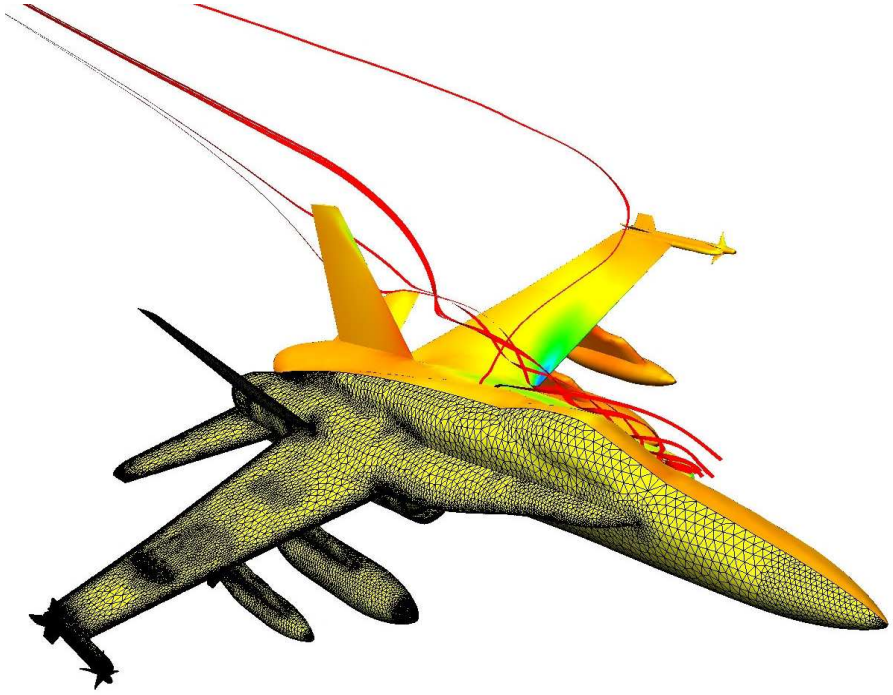

Figure 4: Vortex bursting behavior during buffet analysis of a F/A-18 platform.

tures. This has in turn led into the development of simulation technology that exploits the three-field-based nonlinear aeroelastic formulation and is currently sufficiently efficient and mature to be considered at least as the core technology for a reliable simulation environment for some of the critical flight conditions of a high-performance aircraft. A typical example of the capabilities of this technology is shown in Fig. 4 where vortex bursting is shown during buffet analysis of a F/A-18 platform [56].

The three field, two domains aeroelasticity modeling can be classified to belong in the (2,1,3) region of the space defined in Fig. 1 because it involves one field per domain and the deformation of the fluid domain mesh is introduced as a fictitious entity. On the other hand, if one persists on being literal then it could be classified to belong in the (2,2,3) region.

The Four-Field, Two-Domains Formulation of Aerothermoelastic Models

The previously described formulation, provides an opportunity to examine the realization of the extension of the previously described aeroelastic model from a multi-domain to a multi-field and multi-domain formulation, by incorporating thermal effects that generalized to aerothermoelasticity.

Aerodynamically induced heating can play a dramatic role in the design of of supersonic and hypersonic vehicles due to its potential effect on the stresses, deformations and temperature distributions on the corresponding structures. This can have a direct and significant influence on the material selection and

construction. The end-effects of aerodynamic heating can range from simple deformations that may lead to structural buckling, to potentially serious alteration of the aeroelastic behavior of the aircraft. Early experimental work has demonstrated [76] these effects in an an unexpected – for the time – manner where flutter was induced on a the AGARD wing when exposed to a stagnation temperature of $260C^{\circ}$ while in a wind tunnel providing and airflow of Mach = 2. When the stagnation temperature was reduced to $37C^{\circ}$ then no flutter was observed. The first simulation of of fully coupled fluid-structure-thermal interaction problems has been reported by E. Thornton [77] and has been followed by R. Loehner et al. [78].

The first complete formulation of the nonlinear aerothermoelasticity as a four-field two domains extension of the three field two domain formulation represented by Eqs. (7), was given by Tran and Farhat [79] by the amendment described by:

$$\rho_S c_{pS} \frac{\partial T_S}{\partial t} + \boldsymbol{\nabla}_{\boldsymbol{x}} \cdot (-\tilde{\boldsymbol{\lambda}}_S \boldsymbol{\nabla}_{\boldsymbol{x}} T_S) - \tilde{\boldsymbol{\sigma}}_S \frac{\partial \tilde{\boldsymbol{\epsilon}}}{\partial t} - Q - q_\Gamma = 0, \text{ in } \Omega_S, \tag{10a}$$

$$\rho_S \frac{\partial^2 \boldsymbol{u}_S}{\partial t^2} - \boldsymbol{\nabla}_{\boldsymbol{x}} \tilde{\boldsymbol{\sigma}}_S(\tilde{\boldsymbol{\epsilon}}_S, T_S) = \boldsymbol{b}, \text{ in } \Omega_S \tag{10b}$$

where $c_{pS}, \lambda_S, T_S, Q, q_\Gamma$ are the specific heat, heat conductivity tensor, temperature field, internal heat source, and boundary heat flux of the structure. Equation (10a) expresses the heat conduction evolution in the structure while Eq. (10b) is used in place of Eq. (7b) and is identical to it, except of the fact that the stress tensor in now a function of not only the strain tensor, but also of the temperature field as well.

The boundary conditions for this case are extended to include the thermal boundary conditions given by,

$$T_S = T_F \quad , \text{ on } \Gamma(t), \tag{11a}$$

$$\lambda_S \boldsymbol{\nabla} T_S \boldsymbol{n} = -\lambda_F \boldsymbol{\nabla} T_F \boldsymbol{n}, \text{ on } \Gamma(t), \tag{11b}$$

where the thermal conductivities have been considered assuming isotropic material for the structure and the fluid and therefore they are written in tensor notation.

The four field, two domains aerothermoelasticity modeling can be classified to belong in the (2,2,3) region of the space defined in Fig. 1.

An example of the ability that this formulation is shown in Fig. 5 where the simulated distribution of the aerodynamically induced temperature is shown for the skin surface of the F-16 fighter jet.

CIE-related contributions on the topic of multi-domain applications are limited and are contributed on the application areas of combustion [80, 81], fluid-structure interaction [82, 83], and phase transformation [84, 85].

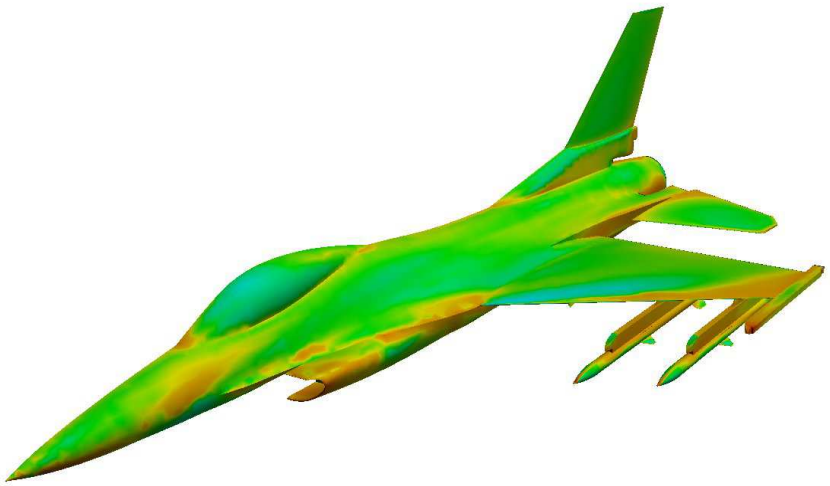

Figure 5: Aerodynamically induced temperature distribution on the skin of the F-16 fighter.

MULTI-SCALE RETROSPECTIVE

To understand the motivating needs for a multi-scale modeling agenda we will compare two engine systems defined in different scales. The size of a jet engine is of order of meters. Its continuum behavior description is traditionally captured by means of partial differential equations, and consequently, discretization methods such as finite elements, finite volume or finite differences can be used to determine the state variable fields associated with it. On the other hand, a rotary motor that drives Salmonella and E. coli bacteria has a diameter of 30 nm. This motor is rotating at approximately 20,000 rpm, consumes about 10-16 W and exhibits an energy conversion efficiency close to 100% [86]. A continuum description for this nano-engine is not equipped to account for predominant surface effects and if applied, it would result in unrealistically stiff behavior. Alternatively, a brute force approach of modeling the rotary motor entirely on atomistic scale would necessitate an impractically high number (billions) of unknowns. Thus, the employment of a multiscale computational paradigm where important atomistic features could be captured at a fraction of computational cost required by atomistic simulation of the entire system [87] becomes a potentially appropriate approach. One of the main barriers in developing such a rigorous discrete-to continuum scale-bridging framework, is the increased uncertainty and complexity introduced by small scales that expose the discrete character of matter constituents.

Application context often determines how extensively multiscale methods can be used. For example, in case of metal matrix composites (MMC) with almost periodic arrangement of fibers, introducing finer scales might be advantageous since the bulk material typically does not follow normality rules and developing a

phenomenological coarse scale constitutive model might be challenging at best. The behavior of each phase is well understood and obtaining the overall response of the material from its fine scale constituents can be obtained using homogenization. On the other hand, in brittle ceramics composites (CMC), the microcracks are often randomly distributed and characterization of their interface properties is difficult. In this case, the use of fine scale models may not be beneficial.

Here we focus on a bridging continuum and discrete scales, which encompasses most of the issues associated with continuum-to-continuum scale bridging. For an excellent exposition of various continuum-to-continuum scale bridging approaches we refer to [88]. In what follows we present a brief description of available methods for multiscale modeling from two perspectives.

The first perspective involves the information passing between models on different scales defined within a range that extends from discrete to continuum formalisms. In addition, the discrete scale is modeled first, such that its gross response is subsequently infused into the continuum scale. Therefore, information follows a one-way path from discrete to continuum scale models. The second perspective involves concurrent modeling of both the discrete and continuous scales. For the sake of comprehensive completeness we refer to the review articles [89, 90] and to a comprehensive study on adaptive control of multiscale models [91].

Multi scale modeling can be classified to belong in the (1-2,1,1-3) region of the space defined in Fig. 1 because it usually involves single field activation of multiple domains over at least two length scales. The two categories of multiscale approaches can be described by extending the system of coupled Eqs. Eq. (1) to include variable indexes for length scale in the form

$$\mathcal{D}_{di}(\hat{q}_{djk}, \hat{p}_{djk}; \dot{\hat{q}}_{djk}, \dot{\hat{p}}_{djk}) = 0, \text{ on } \bigcup_{d=1}^{nlc} \Omega_d, \tag{12}$$

with $k \in [1, nli]$ and $d \in [1, nlc]$, where nli is the number of length scales treated by one of the information-passing multiscale approaches and nlc is the number of concurrent mathematical models represented by different scales.

Information-passing multiscale methods

Calculations at finer scales, are used to evaluate certain quantities (i.e. discrete system state variables) for use in approximate or computational models defined within longer length/time scales in all information-passing multiscale methods. A direct implication of performing calculations in a finer scale is the high computational complexity predicated by the multiplicative effect of the computed quantities for a volume of the material shared by both the finer and the coarser scale models. This type of scale bridging is also known as sequential, serial or parameter passing. However, for nonlinear problems fine and coarse scale models are two-way coupled, i.e., the information continuously flows between the models in different scales. Here we

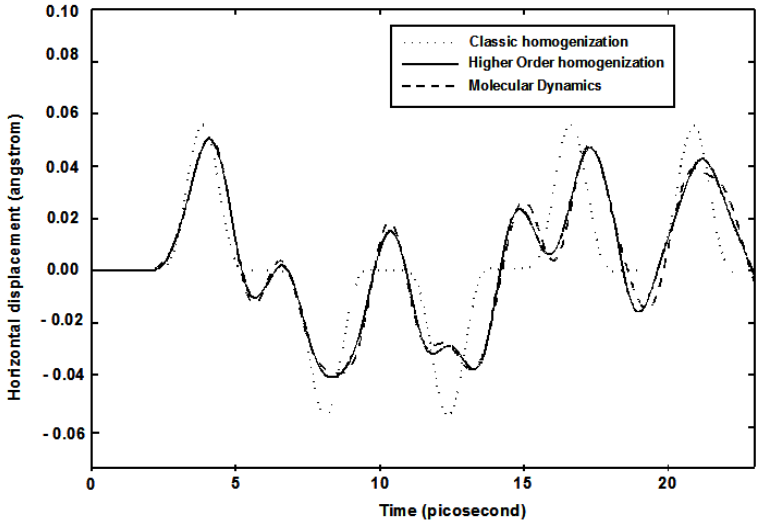

Figure 6: Comparison of GMH with classical (spatial) homogenization and molecular dynamics (MD) simulations.

present several information passing bridging techniques.

Generalized Mathematical Homogenization (GMH): The GMH theory [92, 93] constructs an equivalent continuum description directly from molecular dynamics (MD) equations. In this method the displacement field is constructed as simultaneous asymptotic expansion of multiple space-time scales. This approach allows the decomposition of the coarse scale models to a sequence of discrete unit cell problems and various order continuum problems with multiple scales [93]. The sequence of discrete unit cell problems can be interpreted as molecular statics problems where a unit cell is subjected to various order of macroscopic fields. Continuum equations can be combined to construct a nonlocal continuum description [92, 94, 95], or alternatively, a closed-form solution for slow time scales can be obtained leading to algebraic system of equations with a single time scale [93]. Figure 6 compares the GMH, with spatial homogenization [96] and molecular dynamics simulation for wave propagation in a layered lattice structure [93]. It can be seen that GMH provides a comparable accuracy to MD simulation despite significant reduction in degrees-of-freedom. To this end we note that for the GMH to be valid both the temporal and spatial scales have to be separable. For instance, if the essential events of the faster fine scale model occur on the same time scales as the details of processes computed using the slower coarse model, then the time scales cannot be separated. Likewise, when the wavelength of the traveling signal is of the order of magnitude of the fine scale features, then separation of spatial scales cannot be accomplished.

Quasicontinuum (QC): QC method involves a continuum description where constitutive equations are constructed directly from atomistic considerations rather than from a phenomenological or thermodynamically-based constitutive model. The atomistically enabled constitutive model is adequate as long as continuum fields are varying slowly over a unit cell domain. In its original form [97] the QC method was formulated for

simple Bravais crystals assuming uniform deformation of atoms. In a more general case with heterogeneous interatomic potentials, a unit cell problem has to be solved instead [98]. In this more general scenario, the QC method resembles GMH and as such it can be viewed as an engineering counterpart of the mathematical theory. Note that both the "engineering" and mathematical homogenization methods involve solution of an atomistic unit cell problem and subsequently feeding the continuum problem with effective properties.

Multiscale Enrichment based on the Partition of Unity (MEPU): The MEPU method [99] can be considered as a generalized combination of the GMH [93] and the Partition of Unity [100, 101, 102] methods. MEPU is suitable for enriching coarse scale continuum description or coarse-grained discrete formulations. It is primarily intended to extend the range of applicability of the mathematical homogenization theory to problems where scale separation may not be valid, such as in the case on non-periodic solutions or problems where the coarse solution may rapidly vary over the domain of the unit cell domain. MEPU can be classified in the category of methods that employ hierarchical decomposition of the approximation space. To reduce the computational cost, homogenization-like integration scheme is devised. The value of a function at a gauss point of a coarse scale element is replaced by an average computed over a unit cell domain centered at a Gauss point. It has been proved that the accuracy of the integration scheme is of order $O(1/n)$ where n is the number of unit cells in the coarse scale element domain. The molecular model of a polymer subjected to uniform macroscopic fields the polymer has been modeled using a single MEPU element with nine degrees of freedom per node [22]. The error in L_2 norm of displacements was 2% compared to the 9% when using the QC method.

Variational Multiscale Method (VMS): The VMS method [103], can be viewed as an equivalent coarse scale element builder method. It was originally developed for enriching continuum solutions with fine scale continuum description. Most common implementation of the method assumes the fine scale enrichment to be a residual free bubble vanishing on coarse scale element boundaries. Based on this assumption, the enrichment functions can be condensed out on the element level to give *effective coarse scale elements* as opposed to *effective material properties* as they appear in the GMH approach. Alternatively, a better accuracy can be obtained by enforcing enrichment functions to vanish on the element boundaries in the weak sense. VMS can be easily extended to enriching coarse grained descriptions, such as for instance in QC. According to this scenario the coarse-grained description which amounts to interpolating the solution between the representative atoms, (element nodes in Fig. 7) can be enriched using kinematics of individual atoms in the areas where such enrichment in necessary. Since positions of atoms may not coincide with the coarse scale element boundaries, homogeneous boundary condition of atoms residing in the vicinity close to the element boundaries can be enforced as shown in Fig. 7.

Heterogeneous Multiscale Method (HMM): The foundational idea behind the HMM method is the ap-

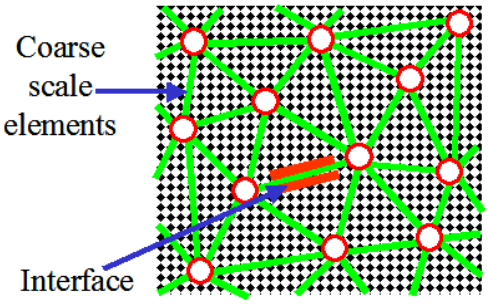

Figure 7: VMS for enriching coarse grained models.

proximation of the coarse scale integrands by data computed from the auxiliary fine scale problem [104]. The auxiliary fine scale problem is an atomistic cell subjected to boundary conditions extracted from the coarse scale solution. HMM can be viewed as a method to construct effective integrands based on the fine scale data as opposed to effective properties in GMH or to effective elements in VMS.

Coarse-Grained Molecular Dynamics (CGMD): The CGMD method develops coarse-grained Hamilton's equations from MD equations under fixed thermodynamic conditions [87, 105]. The representative atoms are enforced to preserve an average position and momenta of the fine scale atoms (similar to those employed in the QC method). The corresponding coarse-grained Hamiltonian is defined as an average of the thermodynamically calibrated fine scale Hamiltonian, in the displacement-momenta space.

Discontinuous Galerkin (DG): The DG method constructs discontinuous enrichment of the displacement field in a manner that resembles mathematical homogenization, but it does not introduce multiple spatial coordinates. This causes a C^{-1} continuous approximation of the solution. To control the errors resulting from the discontinuity the oversampling idea of Babuska [106] is used. A generalization of the DG formulation for embedding fine scale features at the continuum level into coarse scale descriptions was given in [107].

Equation-Free Method (EFM): The fine scale problem is evolved at some sampling points in the coarse scale domain according to EFM [108]. These sampling points are represented by a unit cell in the atomic scale. Unlike the aforementioned information-passing methods the coarse problem is assumed to be unknown in EFM. Once the solution in two subsequent time steps on the fine scale is computed and then restricted to the coarse scale, then the coarse scale solution at $t+\Delta t$ is obtained by projective integration or extrapolation in time domain. The fine-to-coarse scale operators are well defined, but the definition of the information flow from the coarse to the fine scale remains to be a challenge. The EFM may be suitable for complex bio-systems whose coarse scale behavior is often unknown.

Other Information-Passing methods: Several useful information-passing procedures have a semi-empirical nature [109, 110, 111, 112]. A popular example is kinetic Monte Carlo for surface growth, where barriers to adatom motion are computed with density functional theory. Similarly, for discrete dislocation dynamics,

mobilities are computed using atomistic simulations.

Concurrent multiscale methods

A class of multiscale approaches for systems whose behavior depends on physics at multiple scales is presented in thissection. Examples of problems that belong into this category are turbulence, crack propagation, friction, and problems involving nano-devices are prime examples. For the case of fracture the crack tip bond breaking can be described with a quantum-mechanical model of bonding, while the rest of the sample is described with empirical potentials. For the case of friction it might be necessary to describe surface interaction using quantum-chemical approaches while using continuum elasticity to simulate the contact forces. These problems, require that multiple scales have to be simultaneously resolved in different portions of the problem domain. Multiscale methods based on the concurrent resolution of multiple scales are often coined as embedded, concurrent, integrated or hand-shaking multiscale methods. Several domain bridging methods [113, 114, 115, 116], multigrid methods [117, 118, 119, 120, 121, 122, 123] and local [124, 125, 102, 126, 99] are used to communicate the information between the subdomains represented by different mathematical models often defined in various scales.

Matching conditions at the interface between different mathematical models is an aspect of concurrent methods. For example, at the MD/continuum interface, according to MD phonons are generated that are not representable in the continuum region and therefore they might be reflected at the continuum/MD interface. This suggests incorporation of interfaces with phonon absorbing properties. Methos to achieve this include damping [113], Langevin equation [127], precomputing exact absorbing boundary conditions for harmonic potentials [128], approximating exact absorbing boundary conditions and calibrating coefficients to minimize reflection [129], matching the properties of continuum and MD at the interface [130], and the bridging domain method [115, 131]. The refinement of the finite element mesh to atomistic scale at the interface [113] may circumvent the phonon reflection issue. A review of various interface formulations can be found in [114], while concurrent bridging between discrete dislocations and continuum region can be found in [132, 133].

Buildup of temporal interfaces is another important aspect of concurrent bridging. In a typical atomistic-continuum problem the time scale for integrating MD equations is dictated by the interatomic spacing and highly heterogeneous interatomic connections. However, the time step at the continuum scale could be much larger especially because the stiff connections have been homogenized and the spacing between the discrete points (for instance, FE nodes) could be substantially larger. To aleviate this problem temporal interfaces can be built using various multi-time-step methods [134] and local enrichment functions in time domain [135], whereas the space-time interfaces can be constructed using space-time Discontinuous Galerkin

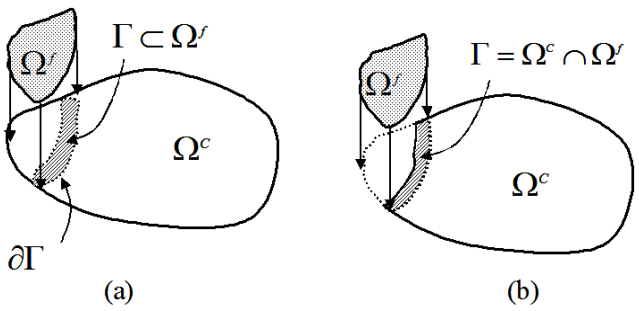

Figure 8: : (a) coexisting domains and (b) overlapping domains.

(DG) method [136]. The multi-step technique developed in [115] preserves stability of time integrators and minimizes spurious reflections from the interfaces as well.

Notable concurrent multiscale methods are the Domain Bridging-based Concurrent Multiscale (DBCM) [113, 115, 131], the Local Enrichment Concurrent Multiscale (LECM) [99, 126, 124, 125], and the Multi-Grid-based Concurrent Multiscale (MGCM) [117, 118, 137]. It is important to make the distinction that these multiscale methods are concerned with a concurrent bridging of dissimilar mathematical models representing different scales, as opposed to the classical domain decomposition, multigrid and enrichment methods, that are primarily concerned with efficient solution of a single scale models.

The basic ideas outlining all of these methods can be described with the help of Fig. 8. In the DBCM approach the fine Ω^f and coarse Ω^c scale subdomains could either overlap or just be coexistent as shown in Fig. 8. The interface, Γ, could be a manifold of the same or lower dimensionality with that of the boundary manifold of course scale $\partial\Omega^c$.

In the MGCM and LECM approaches the subdomains are coexisting (Fig. 8a). The interface, $\Gamma \subset \Omega^f$, is a subdomain in Ω^f defined to be in the vicinity close to the boundary $\partial\Gamma$ as shown in Fig.8a.

The activities in this area in terms of ASME's CIE division has mainly focused only on multigrid methods for mechanics applications [138, 139, 140, 141, 142].

COMPUTATIONAL AND INFORMATION TECHNOLOGY RETROSPECTIVE

Computational technology has played a pivotal role into alleviating the complexity and efficiency associated with the multi-field and multi-domain model generation, computational implementation and predominately systemic simulation. The term will be used here to contain: (i) methods and techniques for model development; (ii) their algorithmic encapsulation and implementation; and (iii) computational machinery and information technology specifically developed to alleviate the complexity and of the associated formalisms in

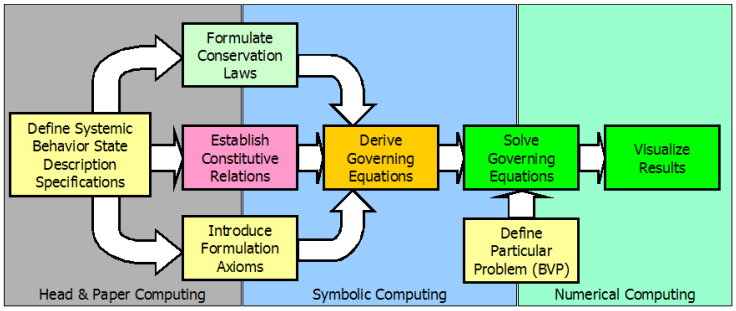

Figure 9: Unified workflow of major modeling and simulation activities along with the computing spaces they are embedded in.

a manner that practitioners of various disciplines (including product development) can extract utility from these models.

In order to describe the context where computational and information technologies are currently contributing relative to the automation they provide on replacing and/or improving human activities, we need some specification of these human activities and their relationship from the M&S perspective. In responding to this need, we present a workflow of the major activities associated with M&S of continuum systems that is capable of carrying the intensions of all multiphysics methods mentioned earlier in this survey. This figure also presents how these activities relate to the "head & paper", "symbolic" and "numerical" types of computing that indicate employment of manual labor, symbolic algebra computing and numerical methods computing respectively. The greatest percentage of the total work done in the computational multiphysics (and even in the single-physics) M&S area falls onto the green activities of numerically solving the appropriate PDEs and visualizing the simulated results after the appropriate formulation of the relevant boundary value problem. This involves the development of algorithmic discretization and integration schemes, their implementations – that often employ distribution of communicating codes over various computational infrastructures –, and execution acceleration methodologies like space and time domain decomposition and distribution over various computational infrastructures. A much less amount of work has been reported in the area of computational automation of the governing equation derivation activity as well as the activities that this process is based on – like the conservation laws tailoring, the constitutive theory derivations and the formulation axioms enrichment activities. Although a significant amount of work exists on the area of constitutive modeling, very little computational automation has been employed in this effort. As our ability to synthesize and process new materials more often than in the past increases, our need to model their behavior also requires accelerating the activity of developing constitutive models and field theories that describe their behavior. This makes the computational automation of this activity increasingly important and almost necessary for the applications of the future.

Traditionally, software tools that integrate algorithms and methodologies, for solving and applying solu-

tions of systems of PDEs representing behavioral models of continuum systems, fall in the category of the "Multidisciplinary Problem Solving Environments" (MPSEs). There are two very distinct schools of thought associated with the philosophy, implementation details and intentions of MPSEs.

One reflects those systems that originated from the domain experts in multiphysics modeling and they are the outgrowth of various codes used for research. These are the codes that usually have the strength that they implement the most recent solution algorithms and methodologies and therefore represent the cutting edge of research capability in the field and can produce the most efficient and accurate results. However, they suffer from the weaknesses of being usable practically only by their developers, since they are – in most cases – undocumented, unstable, buggy, and unverified (in the software sense). Their continuous state of evolution plagues them with unreliability for general purpose problem solving and that renders them practically unusable by the general practitioners from the product design community. On of the best validated and recent representatives of this category has been proven to be the AERO-suite of codes [63, 143].

The second category of MPSEs is originating from the computer science and applied mathematics communities that are also responsible for this naming [144]. These systems are designed to address a wide variety of problems and they have been developed with more emphasis on user-centered utilization. They are also more stable and more well documented. Their problem is that they are not optimized for high performance for specific vertical applications and therefore they are more useful for educational purposes than they are for focused highly targeted and optimized utilization.

The orthogonality between these two categories of MPSEs is apparent and has been identified and the need for bridging the gap has been stressed out and pursued [145, 146].

Essential elements of progress within the context of the first category of MPSEs is subsequently described for the multi-field and multi-domain efforts respectively.

Progress on Computational Multiphysics Modeling Technologies

Progress on Multi-Field Modeling:

During the 1970s and 1980s the emergence and significant evolution of symbolic algebra systems like MACSYMA [147] and Mathematica [148], provided researchers with the opportunity to perform the very rigorous and elaborate computations associated with the constitutive theory derivation process. This was realized early enough by Noor and his colleagues [149] that gave the general the impetus for identifying the opportunity and the challenge associated with this approach by the late 1980s [150]. Representative examples of this practice was given for single-physics formulations for various CFT cases – mostly focused in the area of viscoplasticity – [151, 152, 153, 154].

Progress on Multi-Domain Modeling:

The simultaneous solution of nonlinear fluid, fluid-mesh, and structural equations of motion is computationally intensive since it involves space-time integration of the coupled system of PDEs presented earlier. It has been discussed elsewhere [56] that computational speed – which is essential for production environments – favors implicit integration schemes and large computational steps, which underscores the importance of paying special attention to the numerical stability properties of the scheme designed for time-integrating the coupled fluid/structure equations of motion.

Time-accuracy is another crucial requirement when simulating a nonlinear aeroelastic phenomenon in the time-domain, not only for performance objectives as outlined above, but also for fidelity reasons. In the context of the three-field formulation of nonlinear aeroelastic problems, this is to be understood as a time-accuracy requirement for the solution of the coupled equations 7. However, whether these governing equations are solved by a monolithic, partitioned, strongly-coupled, or loosely coupled algorithm, a more time accurate aeroelastic solution implies a more time-accurate time-stepping during the solution of the semi-discrete fluid equation of motion [56] on dynamic meshes. Typically, a time-integration algorithm for solving the ALE fluid equation is constructed by combining a preferred time-integrator for fluid-grid computations and an ad-hoc procedure for evaluating the geometric quantities arising from the ALE formulation. Unfortunately, such an approach for designing an ALE time-integrator does not necessarily preserve the order of time-accuracy of its fixed-grid counterpart. This issue has been rarely recognized in the literature and among practitioners of nonlinear computational aeroelasticity. To address this issue, two different methods for extending to moving grids a preferred time-integrator, while preserving its order of time-accuracy established on fixed grids were presented [155, 64].

Methods and algorithmic implementations for achieving both numerical stability and time accuracy have been two of many features associated with the AERO suite of codes [63, 143] that originated development at university of Colorado at Boulder and continuing at Stanford university. Besides this system of codes various other software tools and systems for the parallel finite element analysis of single discipline and multidisciplinary problems, including the Finite Element Tear and Interconnect (FETI) solver [156] and the TOP/DOMDEC visualizer and mesh partitioner [157] have been developed and are very popular in production engineering environments.

Progress on Multi-Scale Modeling:

To our knowledge as of today, there is no general-purpose multiscale code in existence. Nevertheless, commercial packages, such as ANSYS, ABAQUS, DYNA among others, can be utilized to implement information-passing multiscale algorithms through user-defined material models (USERMAT/UMAT) routines. By this approach, the custom-made UMAT makes calls to either a user-provided numerical code or to a commercial code itself. The former, has been used for modeling composite material and structures [158, 159], while the

latter has been employed for resolving multiple temporal scales associated with fatigue life predictions [160]. Multiscale enrichment schemes [99] can be implemented through a user-defined element (UEL) routines provided by most of the commercial finite element codes. By this approach finite elements with arbitrary number of degrees-of-freedom representing fine scale enrichment features have been developed and implemented in ABAQUS [99]. On the discrete level, the Network for Computational Nanotechnology [161] developed multiscale software with emphasis on micro-electronics. Coventor [162] is developing integrated multiscale tools for MEMS and micro-fluidic devices with emphasis on continuum modeling tools. An integrated multiscale framework that links continuum and discrete codes is currently under development at Rensselaer.

Regarding the progress associated with the second of the two categories of MPSEs as described earlier, that originate from Computational Science groups are: the GasTurbnLab [163, 164] MPSE for gas turbine engine design, the WebPDELab [165] PSE for solving systems of PDEs, user specific domain knowledge efforts have also been implemented to empower users in the selection of need-based scientific software for modeling and solving physical problems such as PYTHIA-II [166]. The most comprehensive contribution on this area has been performed at Purdue University with many additional agent- and non-agent based systems [167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177].

Information Technology Infrastructure Progress

The plethora of available choices on computational infrastructure (hardware, software, networking) along with specific domain of application and user specific backgrounds and needs have introduced a large number of research issues associated with the computational implementation of Multidisciplinary Problem Solving Environments (MPSEs). The most important of these issues are: (1) ability and optimization for computation over distributed resources, (2) ability for dynamic migrating component distribution, (3) adaptive modeling capability, (4) user dependent customization, (5) collaborative knowledge representation and interactivity, (6) dealing with heterogeneity of legacy and new code, and finally (7) ability to sustain component fault tolerance.

During the last decade there was a strong current of efforts that attempted to address as many as of the issues as possible. These systems can be classified according to particular features of their use by the following categories:

(1) Systems for interactive program construction: Systems in this category provide support for interactive program construction based on a two dimensional data-flow diagramming approach that in many cases maps onto the workflow diagram representing the sequencing of activities of the researcher when designing, building and executing all the necessary operations for obtaining final simulation results. Noted systems in this category are SCIRun [178],

(2) Systems for remote application configuration and deployment: These systems use existing high performance back-end resources and provide powerful visual authoring toolkits to configure and deploy distributed applications. Therefore, they are an extension of the previous category in that computational modules need not be restricted within one execution environment within one machine. The CoG Kits [179] provide commodity access to the Globus [180] metacomputing environment. The WebFlow [181] and Gateway [182] systems provide support for configuring, deploying and analyzing distributed applications. More recently systems like ICENI [183], Taverna and MyGrid [184], Teuta and Askalon [185, 186], and finally Kepler [187].

(3) Systems for interactive run-time steering and control:

Event based steering systems: In these systems, monitoring and steering actions are based on low-level system "events" that occur during the course of program execution. The Progress [188] and Magellan [189] systems use this approach and require a server process executing in the same address space as the application to enable interaction. The Computational Steering Environment (CSE) [190] uses a data manager as a blackboard for communicating data values between the application and the clients.

Systems with high-level abstractions for steering and control: The Mirror Object Steering System (MOSS)[191] provides a high-level model for steering applications and the DISCOVER [192] control network extends this approach.

Collaboration groupware: These systems primarily focus on enabling collaboration but occasional they can also provide support for problem solving [192].

Some efforts to bridge the gap between the two schools of thought for MPSEs while satisfying the available computational technology and focusing on the multiphysics characteristics, – but for the application context aircraft design – have originated by the proposed architecture and initial implementations of Virtual Wind Tunnel Environment (VWT) based on nonlinear material behavior [193, 194, 195]. These efforts have culminated into the even more recent effort of the Data Driven Environment for Multiphysics Applications (DDEMA) [145, 47, 196, 197, 146] that extended the VWT motivations to include other multiphysics design contexts such that of a combination of sensor and computational grids for modeling fire dynamics evolution and and implementing the first responders decision support solutions. Some of this work has also been reported during the CIE activities [45].

Additional work done under the auspices of the CIE division activities has been performed in various areas that although they were not explicitly related to multiphysics efforts, nevertheless they were very supportive on many fundamental contexts that are always present in single-physics M&S efforts. Thus, many (if not all) of the efforts of the Finite Element Techniques and Computational Technologies (CTFE) subcommittee that has been recently expanded its scope and was renamed to Computational Technologies for Engineering Science Applications (CTESA) fall in this category. In particular, a significant amount of progress has been

reported to various PDE discretization techniques including Finite Element analysis methods and associated technologies. In the period between 1987 and 2004 the CIE conference proceedings include 15 papers in the combustion modeling area, 89 papers in the computational mechanics area, 10 papers in the computational fluid dynamics area, and 24 papers in the flow and heat transfer area.

Heterogeneity of involved codes, software and hardware architectures continuously strains the data exchange capabilities of modelers utilizing the above mentioned technologies. This need has been recognized and particular efforts have been experienced within CIE to develop and utilize technologies that contribute to intra- or inter-application integration and data exchange transparency [198, 199].

FUTURE DIRECTIONS

The history of predicting the future evolution of technology has been replete from famous disappointments and failures. In 1899 W. Thomson (Lord Kelvin) asserted that "radio has no future", "heavier than air flying machines are impossible", and "X-rays will prove to be a hoax" [200]. In 1943 IBM's T. Watson expressed that "I think there is a world market for maybe five computers" [200]. Their future has been our past for a long time, enough for us to know that these and many other examples demonstrate how easily very capable researchers and technologists – with distinguished domain expertise – can be proven wrong.

Therefore, in an effort to avoid similar disappointments, we are going to avoid far reaching predictions relative to the topic of this survey and we shall rather focus on the emerging and continuing trends. However, we will not refrain from expressing a short outline on where we feel it would be wiser that the future of M&S modeling evolves.

Arguably the one certainty in our considerations about the future will have to take into account three fundamentally undeniable driving factors. The first one is that computational technology will continue improving in anticipated and unanticipated manner. We call this factor the "technology opportunity". The second one refers to the product development and operation economic pressures for reducing total cost of ownership and increasing return on investment. We call this factor the "economic realism". The third one refers to the ever increasing need for holistic cradle-to-grave product development of non-simplified full and detailed complete systems, tailored for maximum efficiency in supporting multidisciplinary missions and needs. We call this factor "technical realism" factor. It is characteristic that any combination of two of these three factors is antagonistic to the remaining one factor. This realization has been referred to as the "principle of technological aggravation" [201] and has been recognized as the nemesis of technology products mostly from the business perspective.

Defeating this "principle" defines implicitly the context of where we feel things might evolve. Practices, technologies, methodologies, algorithms, software, hardware, simulations, and models that contribute to-

wards product development of multiphysics systems, must be able to allow simultaneous satisfaction of the three factors mentioned.

In particular, we anticipate that instead of trying to improve multiphysics product development from each one of these factors' perspective separately, the practices of the future should consider the holistic context of the problem and the counter-activity between the factors . Below we describe specialized trends from each one of the three areas for multiphysics system product development.

For multi-field M&S perspective, it is essential that experimentally-based massive and multi-dimensional data-gathering to drive automated modeling via the support of extensive symbolic-algebra machinery implementing theorem proving methods and inverse methods via generalized global optimization techniques, will be a potential area of evolution. This will not only increase confidence of model prediction (since models will be based on measured data expressing solid quantification of behavioral aspects of the respective physical systems), but it will also help managing representational complexity of associated models and reduce the time of development of these models as well.

For multi-domain M&S perspective, it is inevitable that the evolution of computational power provides opportunities for increasing the number of domains and fields that participate in any model formulations of the future for more comprehensive physical problems. Reduced order modeling techniques in conjunction of precomputation methodologies for simulation synthesis, will improve our ability to perform real-time or near-real-time simulation of very large and complex systems. Combining parallelism in space and time for attacking integration of the PDEs for very large problems will be extended from single- to multi-physics formulations, thus further contributing to computational efficiency.

For the multi-scale M&S perspective, it is essential that two particular issues are addressed globally and in harmony with the previous two areas. First, connections have to be established between system manufacturing processes (i.e. material processing) and the various scales of modeling, if we want to extend the idea of "materials by design" to the idea of "multiphysics systems by design" so it would become possible to tailor manufacturing processes to desired performance characteristics along all scale levels. Secondly, scale modeling coupling has to be extended such equivalence of behaviors in various scale levels can be formally proven to allow intra-scalar parameter identification through data-driven model formation from experiments within all possible scales.

Another direction applicable to all three multiphysics perspectives is the ever important measures against maintenance of degrading multiphysics systems. Clearly, nonlinear dissipative modeling will become more and more prevalent in order to allow aging conditions for automated maintenance of multiphysics systems important to most if not all infrastructure, industrial and defence sectors. Systemic in-line processing and self-healing technologies and prototypes may appear in the next 10 years to address the general maintenance

issue associated with the chronic degradation of various systems leading to their multi-functional aging.

In terms of the computational technology associated with the generation, management and exploitation of M&S approaches, in conjunction with the dynamic and fast evolution of technology, it is expected that: (1) additional contexts of interest will become a part of the holistic design process, to address not only the concerns of the various stake-holders associated with the creation and utilization of multiphysics systems; (2) will provide some permanent knowledge representations that either remain common for all interested parties or are dynamically transformable to match the user customization needs without costly replication of effort. Independence of point of view

In the immediate future we anticipate technologies that contribute to intra- or inter-application integration and data exchange transparency will be developed and evolved as more and more contemporary tools facilitate their exploitation from third party users.

The recently announced initiative on "Dynamic Data Driven Application Systems" by the National Science Foundation [202] is a clear indicator that these trends are not only anticipated but are fostered as well.

CONCLUSIONS

In the present paper we have defined the context space of multiphysics applications from the M&S perspective in terms of the number of fields domains and scales involved. A survey of activities for each one of these areas was presented accompanied by a retrospective on the computational technologies involved for M&S. Finally, a near future description of the anticipated direction of research concludes the main part of the present paper. Special attention has been given into outlining the contributions of ASME's CIE division activities mostly through the conferences held from 1987 until today.

In closing, it should be mentioned that the efforts by the CIE division of ASME have demonstrated an open minded attitude that has been extremely beneficial for the wide audiences and has exposed many technologists to many of the issues mentioned or implied in the present paper.

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