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Partitioned analysis of coupled mechanical systems

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Abstract

This is a tutorial article that reviews the use of partitioned analysis procedures for the analysis of coupled dynamical systems. Attention is focused on the computational simulation of systems in which a structure is a major component. Important applications in that class are provided by thermomechanics, fluid–structure interaction and control–structure interaction. In the partitioned solution approach, systems are spatially decomposed into partitions. This decomposition is driven by physical or computational considerations. The solution is separately advanced in time over each partition. Interaction effects are accounted for by transmission and synchronization of coupled state variables. Recent developments in the use of this approach for multilevel decomposition aimed at massively parallel computation are discussed.

Keywords: Coupled systems; Multiphysics; Partitioned analysis; Staggered solution; Parallel computation; Fluid–structure interaction

1. Introduction

The *American Heritage Dictionary* lists eight meanings for *system*. By itself the term is used here in the sense of "a functionally related group of components forming or regarded as a collective entity". This definition uses "component" as a generic term that embodies "element" or "part", which connote simplicity, as well as "subsystem", which connotes complexity.

We restrict attention to *mechanical* systems, and in particularly those of importance in Aerospace, Civil and Mechanical Engineering. The downplaying of systems of interest in Physics, Chemistry and Electrical Engineering does not imply restriction in methodology extension. It is simply that less experience is available as regards the use of the methods described here.

1.1. System decomposition

Systems are analyzed by *decomposition* or *breakdown*. Complex systems are amenable to many kinds of decomposition chosen according to specific analysis or design objectives. This article focuses on decompositions called *partitions* that are suitable for computer simulation. Such simulations aim at describing or predicting the *state* of the system under specified conditions viewed as external to the system. A set of states ordered according to some parameter such as time or load level is called a *response*.

System designers are not usually interested in detailed response computations per se, but on project goals such as cost, performance, lifetime, fabricability, inspection requirements and satisfaction of mission

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objectives. The recovery of those overall quantities from simulations is presently an open problem in computer system modeling and one that is not addressed here.

The term *partitioning* identifies the process of *spatial* separation of a discrete model into interacting components generically called *partitions*. The decomposition may be driven by physical, functional, or computational considerations. For example, the structure of a complete airplane can be decomposed into substructures such as wings and fuselage according to *function*. Substructures can be further decomposed into submeshes or subdomains to accommodate parallel *computing* requirements. Subdomains are composed of individual elements. Going the other way, if that flexible airplane is part of a flight simulation, a top-level partition driven by *physics* is into fluid and structure (and perhaps control and propulsion) models. This kind of multilevel partition hierarchy: coupled system, structure, substructure, subdomain and element, is typical of present practice in modeling and computational technology.

The present paper focuses on the top decomposition level, which is driven primarily by physics or function. Computational partitions are briefly covered in Section 6.

1.2. Coupled system terminology

Because coupled systems can be studied by many people from many angles, terminology is far from standard. The following summary is one that has evolved for the computational simulation, and does reflect personal choices. Most of the definitions follow usage introduced in a 1983 review article [1]. Casual readers may want to skim the following material and return only for definitions.

A *coupled system* is one in which physically or computationally heterogeneous mechanical components interact dynamically. The interaction is multiway in the sense that the response has to be obtained by solving *simultaneously* the coupled equations which model the system. "Heterogeneity" is used in the sense that *component simulation benefits from custom treatment*.

As noted above the decomposition of a complex coupled system for simulation is *hierarchical* with two to four levels being common. At the first level one encounters two types of subsystems, embodied in the generic term *field*:

Physical subsystems. Subsystems are called *physical fields* when their mathematical model is described by field equations. Examples are mechanical and non-mechanical objects treated by continuum theories: solids, fluids, heat, electromagnetics. Occasionally those components may be intrinsically discrete, as in actuation control systems or rigid-body mechanisms. In such a case the term "physical field" is used for expediency, with the understanding that no spatial discretization process is involved.

Artificial subsystems. Sometimes artificial subsystems are incorporated for computational conveniency. Two examples: dynamic fluid meshes to effect volume mapping of Lagrangian to Eulerian descriptions in interaction of structures with fluid flow, and fictitious interface fields, often called "frames", which facilitate information transfer between two subsystems.

A coupled system is characterized as two-field, three-field, etc., according to the number of different fields that appear in the first-level decomposition.

For computational treatment of a dynamical coupled system, fields are discretized in space and time. A *field partition* is a field-by-field decomposition of the *space* discretization. A *splitting* is a decomposition of the *time* discretization of a field within its time step interval. See Fig. 1. In the case of static or quasi-static analyses, actual time is replaced by pseudo-time or some kind of control parameter.

Partitioning may be *algebraic* or *differential*. In algebraic partitioning the complete coupled system is spatially discretized first, and then decomposed. In differential partitioning the decomposition is done first and each field then discretized separately.

Differential partitioning often leads to non-matched meshes, as typical of fluid–structure interaction (Fig. 2), and handles those naturally. Algebraic partitioning was originally developed for matched meshes and substructuring (Fig. 3), but recent work has aimed at simplifying the treatment of non-matched meshes through frames [2,3].

A property is said to be *interfield* or *intrafield* if it pertains collectively to all partitions, or to individual partitions, respectively. A common use of this qualifier concerns parallel computation. *Interfield parallelism* refers to the implementation of a parallel computation scheme in which all partitions can be concurrently

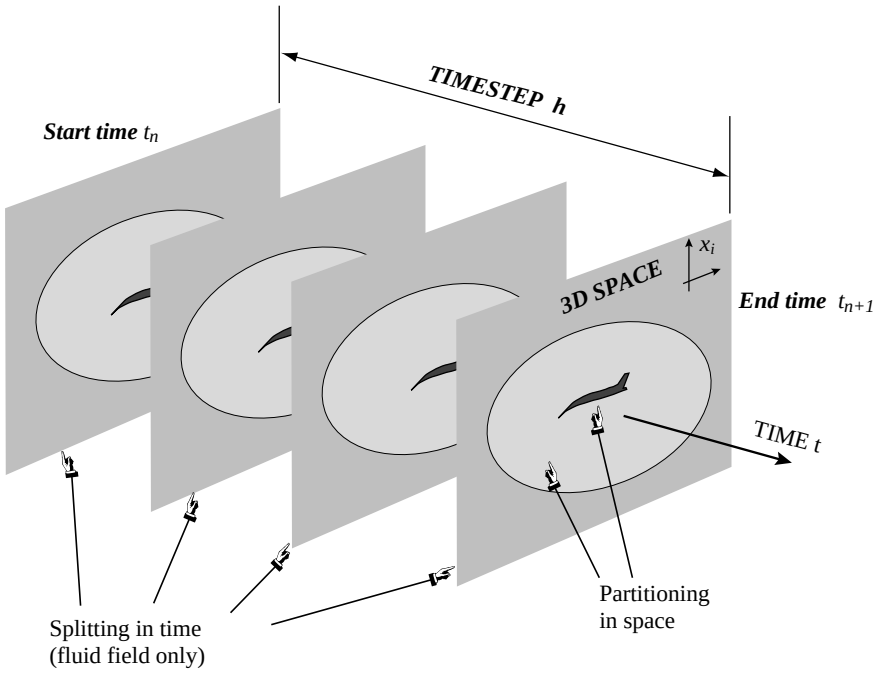

Fig. 1. Decomposition of an aeroelastic FSI coupled system: *partitioning* in space and *splitting* in time. 3D space is shown as "flat" for visualization convenience. Spatial discretization (omitted for clarity) may predate or follow partitioning. Splitting (here for fluid only) is repeated over each timestep and obeys time discretization constraints.

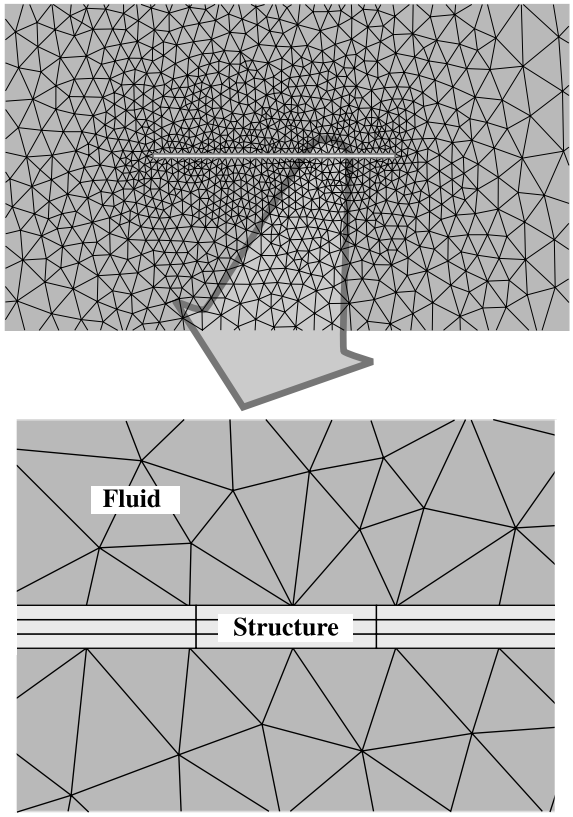

Fig. 2. Differential partitioning was originally developed for fluid–structure interaction problems, in which non-matched meshes occur naturally.

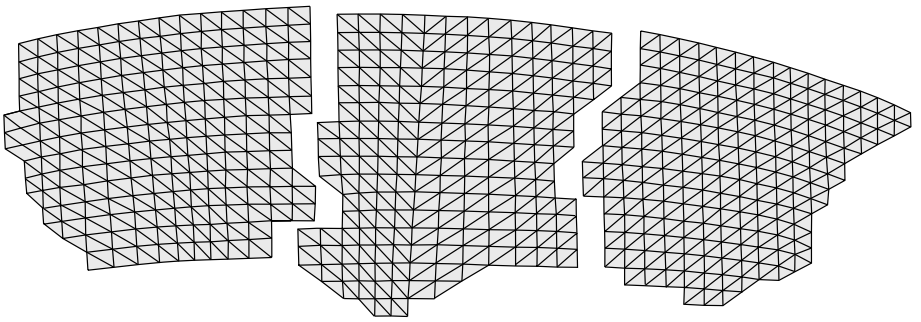

Fig. 3. Algebraic partitioning was originally developed to handle matching meshes, as typical of structure–structure interaction.

processed for time-stepping. *Intrafield parallelism* refers to the implementation of parallelism for an individual partition using a second-level decomposition; for example into substructures or subdomains.

1.3. Examples

Experiences reported here come from systems where a *structure* is one of the fields. Accordingly, all of the following examples list structures as one of the field components. The number of interacting fields is given in parenthesis.

- Fluid–structure interaction (2);
- thermal–structure interaction (2);
- control–structure interaction (2);
- control–fluid–structure interaction (3);
- fluid–structure–combustion–thermal interaction (4).

When a fluid is one of the interacting fields a wider range of computational modeling possibilities opens up as compared to, say, structural or thermal fields. For the latter finite element discretization methods can be viewed as universal in scope. On the other hand, the range of fluid phenomena is controlled by several major physical effects such as viscosity, compressibility, mass transport, gravity and capillarity. Incorporation or neglect of these effects gives rise to widely different field equations as well as discretization techniques.

For example, the interaction of an acoustic fluid with a structure in aeroacoustics or underwater shock is computationally unlike that of high-speed gas dynamics with an aircraft or rocket, or of flow through porous media. Even more variability can be expected if chemistry and combustion effects are considered. Control systems also exhibit modeling variabilities that tend not to be so pronounced, however, as in the case of fluids.

The partitioned treatment of some of these examples is discussed further in subsequent sections.

1.4. Splitting and fractional step methods

Splitting methods for the equations of mathematical physics predate partitioned analysis by two decades. In the American literature they can be originally traced to the development by 1955 of alternating direction methods by Peaceman, Douglas and Rachford (see e.g. [4,5]). A similar development was independently undertaken in the early 1960s by the Russian school led by Bagrinovskii, Godunov and Yanenko, and eventually unified in the method of fractional steps [6]. The main computational applications of these methods have been the equations of gas dynamics in steady or transient forms, discretized by finite difference methods. They are particularly suitable for problems with layers or stratification, for example atmospheric dynamics or astrophysics, in which different directions are treated by different methods.

The basic idea is elegantly outlined in the monograph by Richtmyer and Morton [7]. Suppose the governing equations in divergence form are $\partial W/\partial t = AW$, where the operator A is split into

$A = A_1 + A_2 + \cdots + A_q$. Chose a time difference scheme and then replace A successively in it by $qA_1, qA_2, \ldots$, each for a fraction h/q of the temporal stepsize h. Then a multidimensional problem can be replaced by a succession of simpler (e.g., one-dimensional) problems. Splitting may be *additive*, as in the foregoing example, or *multiplicative*. Since the present article focus on partitioned analysis, the discussion of these variations falls beyond its scope.

Comparison of such methods with partitioned analysis makes clear that little overlap occurs. Splitting is appropriate for the treatment of a field partition such as a fluid, if the physical structure of such partition display strong directionality dependencies. Consequently splitting methods are seen to pertain to a lower level of a top-down hierarchical decomposition.

1.5. Computational multiphysics

Recently the term *multiphysics* has gained prominence within computational physics and mechanics. This subject can be viewed as being more general than coupled mechanical systems in two senses:

- It embraces problems of importance in the physical sciences, which may go beyond engineering technology. For example, electromagnetic and chemistry phenomena.
- Wider ranges of interacting length and time scales are addressed. This may leads to multiple models of the same field, which coexist in space and time. Instances of this class of problems occur in computational micromechanics, progressive fracture and damage, and fluid turbulence.

Given this wider scope, one must be cautious in claiming that a certain partitioned approach, proven useful for a class of coupled systems, is a panacea for multiphysics. Merits and disadvantages must be assessed on a case-by-case basis. The volume coupling inherent in multiple scale problems may in fact hinder the use of partitioned analysis.

2. Coupled system simulation

2.1. Scenarios

Because of their variety and combinatorial nature, the simulation of coupled problems rarely occurs as a predictable long-term goal. Some more likely scenarios are as follows.

Research project. Two or more persons in a research group develop expertise in modeling and simulation of two or more isolated problems. They are then called upon to pool that disciplinary expertise into a coupled problem.

Product development. The design and verification of a product requires the concurrent consideration of interaction effects in service or emergency conditions. The team does not have access, however, to software that accommodates those requirements.

Software house. A company develops commercial application software targeted to single fields as isolated entities: a CFD gas-dynamics code, a structure FEM program and a thermal conduction analyzer. As the customer base expands, requests are received for allowing interaction effects targeted to specific applications. For example the CFD user may want to account for moving rigid boundaries, then interaction with a flexible structure, and finally to include a control system.

The following subsection discusses three approaches to these scenarios.

2.2. Approaches

To fix the ideas we assume that the simulation calls for *dynamic analysis* that involves following the time evolution of the system. (Static or quasi-static analyses can be included by introducing a pseudo-time history parameter.) Furthermore the modeling and simulation of isolated components is supposed to be well understood. The three approaches to the simulation of the coupled system are:

Field elimination. One or more fields are eliminated by techniques such as integral transforms or model reduction, and the remaining field(s) treated by a simultaneous time-stepping scheme.

Monolithic or simultaneous treatment. The whole problem is treated as a monolithic entity, and all components advanced simultaneously in time.

Partitioned treatment. The field models are computationally treated as isolated entities that are separately stepped in time. Interaction effects are viewed as forcing effects that are communicated between the individual components using prediction, substitution and synchronization techniques.

Field elimination is restricted to special linear problems that permit efficient decoupling. It often leads to higher order differential systems in time, or to temporal convolutions, which can be the source of numerical difficulties.

Both the monolithic and partitioned treatment are general in nature. No technical argument can be made for the overall superiority of either. Their relative merits are not only problem dependent, but are interwined with human factors as discussed below.

2.3. Parting can be sweet or sorrow

The keywords that favor the partitioned approach are: customization, independent modeling, software reuse, and modularity.

Customization. This means that each field can be treated by discretization techniques and solution algorithms that are known to perform well for the isolated system. The hope is that a partitioned algorithm can maintain that efficiency for the coupled problem if (and that is a big if) the interaction effects can be also efficiently treated. As discussed in Section 5, in the original problem that motivated the partitioned approach that happy circumstance was realized.

Independent modeling. The partitioned approach facilitates the use of non-matching models. For example in a fluid–structure interaction problem the structural and fluid meshes need not coincide at their interface. This translates into project breakdown advantages in analysis of complex systems such as aircraft. Separate models can be prepared by different design teams, including subcontractors that may be geographically distributed.

Software reuse. Along with customized discretization and solution algorithms, customized software (private, public or commercial) may be available. Furthermore, there is often a gamut of customized peripheral tools such as mesh generators and visualization programs. The partitioned approach facilitates taking advantage of existing code. This is particularly suitable to academic environments, in which software development tends to be cyclical and loosely connected from one project to another.

Modularity. New methods and models may be introduced in a modular fashion according to project needs. For example, it may be necessary to include local nonlinear effects in an individual field while keeping everything else the same. Implementation, testing and validation of incremental changes can be conducted in a modular fashion.

These advantages are not cost free. The partitioned approach requires careful formulation and implementation to avoid serious degradation in stability and accuracy. Parallel implementations are particularly delicate. Gains in computational efficiency over a monolithic approach are not guaranteed, particularly if interactions occur throughout a volume as is the case for thermal and electromagnetic fields. Finally, the software modularity and modeling flexibility advantages, while desirable in academic and research circles, may lead to anarchy in software houses.

In summary, circumstances that favor the partitioned approach for tackling a new coupled problem are: a research environment with few delivery constraints, access to existing software, localized interaction effects (e.g. surface versus volume), and widespread spatial/temporal component characteristics. The opposite circumstances: commercial environment, rigid deliverable timetable, massive software development resources, global interaction effects, and comparable length/time scales, favor a monolithic approach.

The remainder of this article focuses on the partitioned approach. It presents the essentials for a simple problem, and then outlines the application of the methodology to more complex situations using case studies.

3. The basic idea

Consider the two-way interaction of two scalar fields, X and Y, sketched in Fig. 4. Each field has only one state variable identified as $x(t)$ and $y(t)$, respectively, which are assumed to be governed by the first-order differential equations

$$3\dot{x} + 4x - y = f(t), \quad \dot{y} + 6y - 2x = g(t) \tag{1}$$

in which $f(t)$ and $g(t)$ are the applied forces. Treat this by Backward Euler integration in each component:

$$x_{n+1} = x_n + h\dot{x}_{n+1}, \quad y_{n+1} = y_n + h\dot{y}_{n+1}, \tag{2}$$

where $x_n \equiv x(t_n)$, $y_n \equiv y(t_n)$, etc. At each time step $n = 0, 1, 2, \ldots$ one gets

$$\begin{bmatrix} 3+4h & -h \\ -2h & 1+6h \end{bmatrix} \begin{bmatrix} x_{n+1} \\ y_{n+1} \end{bmatrix} = \begin{bmatrix} hf_{n+1} + 3x_n \\ hg_{n+1} + y_n \end{bmatrix} \tag{3}$$

in which $\{x_0, y_0\}$ are provided by the initial conditions. In the monolithic or simultaneous solution approach, (3) is solved at each timestep, and that is the end of the story.

3.1. Staggering

A simple partitioned solution procedure is obtained by treating (3) with the following *staggered partition* with prediction on y:

$$\begin{bmatrix} 3+4h & 0 \\ -2h & 1+6h \end{bmatrix} \begin{bmatrix} x_{n+1} \\ y_{n+1} \end{bmatrix} = \begin{bmatrix} hf_{n+1} + 3x_n + y^{\mathrm{P}}_{n+1} \\ hg_{n+1} + y_n \end{bmatrix}. \tag{4}$$

Here y^{P}_{n+1} is a *predicted value* or simply the *predictor*. Two common choices are $y^{\mathrm{P}}_{n+1} = y_n$ and $y^{\mathrm{P}}_{n+1} = y_n + h\dot{y}_n$. The basic solution steps are displayed in Fig. 5. The main achievement is that systems X and

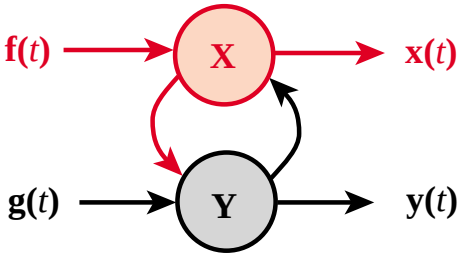

Fig. 4. The red and the black.

BASIC STEPS

1. (**P**) **Predict**: $y^{P}_{n+1} = y_n + h\dot{y}_n$ *(for example)*
2. (**Ax**) **Advance** x: $x_{n+1} = \dfrac{1}{3+4h}(h f_{n+1} + 3x_n + y^{P}_{n+1})$
3. (**S**) **Substitute:** $x_{n+1} = x_{n+1}$ *(trivial here)*
4. (**Ay**) **Advance** y: $y_{n+1} = \dfrac{1}{1+6h}(h g_{n+1} + y_n + 2x_{n+1})$

Fig. 5. Basic steps of a red/black staggered solution.

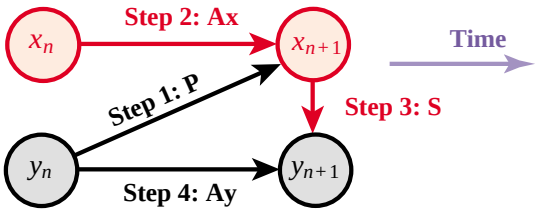

Fig. 6. Interfield + intrafield time-stepping diagram of the staggered solution steps listed in Fig. 3.

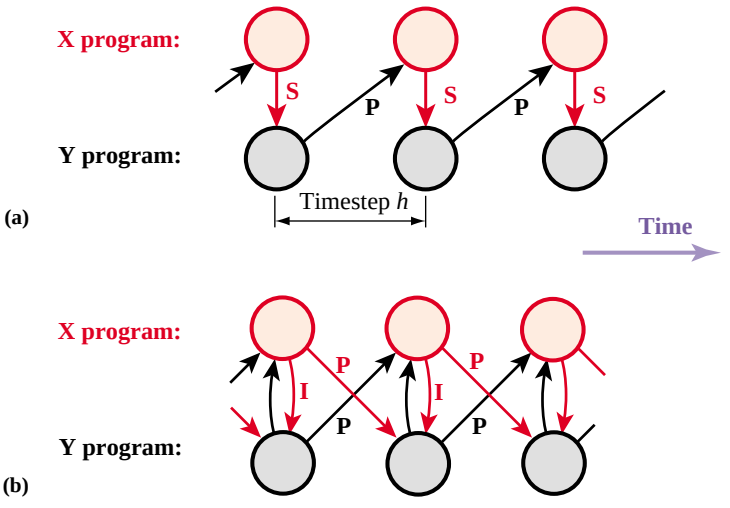

Fig. 7. Interfield time-stepping diagrams: (a) sequential staggered solution of example problem, (b) naive modification for parallel processing.

Y can be now solved *in tandem*. A state–time diagram of these steps, with time along the horizontal axis, is shown in Fig. 6.

Suppose that fields X and Y are handled by two communicating programs called the Single Field Analyzers, or SFAs. If the intrafield advancing arrows are suppressed, we obtain a zigzagged picture of interfield data transfers between the X program and the Y program, as depicted in Fig. 7(a). This graphical interpretation motivated the name *staggered solution procedure* [8].

3.2. Concerns

In *linear* problems the first concern with partitioning should be degradation of time-stepping *stability* caused by prediction. In the foregoing example this is not significant. The spectral analysis presented in Appendix A, which embodies (4) as instance, shows that staggering does not harm stability, or even accuracy, if the predictor is chosen appropriately. In fact, staggered procedures are extremely effective for coupled first-order parabolic systems. But for more general problems, particularly those modeled by oscillatory second-order ODEs, the reduction of stability can become serious or even catastrophic.

Prediction could be done on the y field, again leading to a zigzagged diagram with substitution on x. The stability of both choices can be made identical by appropriately adjusting predictors.

Once satisfactory stability is achieved, the next concern is *accuracy*. This is usually degraded with respect to that attainable by the monolithic scheme. In principle this can be recovered by *iterating* the state between the fields. Iteration is done by cycling substitutions at the same time station. However, *interfield iteration generally costs more than cutting the timestep* to attain the same accuracy level. If, as often happens, the monolithic solution is more expensive than the staggered solution for the same timestep, we note the emergence of a tradeoff.

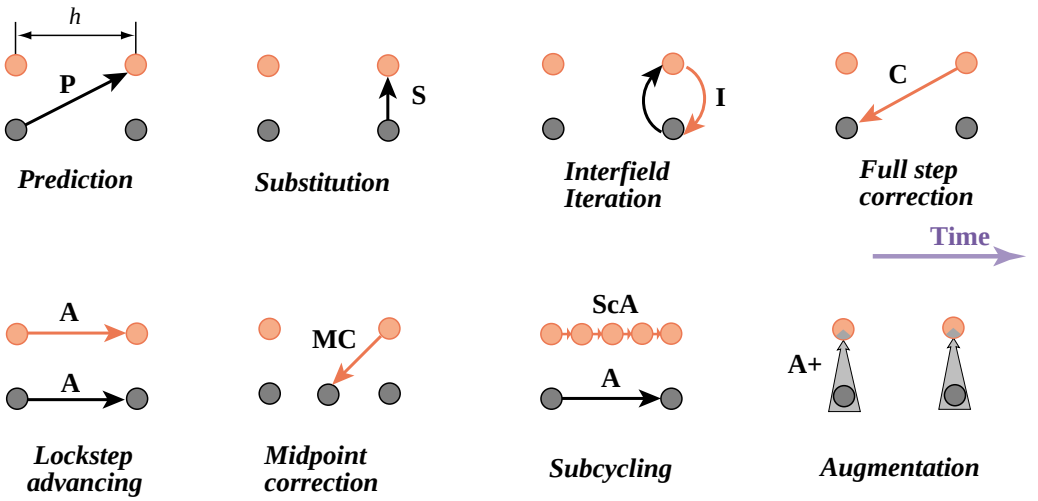

Fig. 8. Devices of partitioned analysis time-stepping.

In strongly *nonlinear* problems, such as fluid flow, stability and accuracy tend to be interwined (since numerical stability is harder to define) and they are usually considered together in method design. The expectation is for a method that operates well at a reasonable timestep.

Examination of Fig. 7(a) shows than this simple staggered scheme is unsuitable for interfield parallelization because programs must execute in a strictly *serial* fashion: first X, then Y, then X, etc. This was of little concern when the method was formulated in the mid 1970s, because all computers – with the exception of an exotic machine known as the ILLIAC IV – were then sequential.

The variant sketched in Fig. 7(b) permits both programs to advance their internal state concurrently, which fits a parallel computer better. More practical parallel schemes, which do not require prediction on both fields, have been developed in recent years and are discussed in Section 6.

3.3. Devices of partitioned analysis

As the simple example makes clear, partitioned analysis requires the examination of alternative algorithm and implementation possibilities as well as the study of tradeoffs. Fig. 8 displays, using interfield time-stepping diagrams, the main "tools of the trade". Some devices such as prediction, substitution and iteration have been discussed along with the foregoing example. Others will emerge in the application problems discussed in Sections 5 and 6.

4. Background

The partitioned treatment of coupled systems involving structures emerged independently in the mid 1970s at three locations: Northwestern University by T. Belytschko and R. Mullen, Cal Tech by T.J.R. Hughes and W.K. Liu, and Lockheed Palo Alto Research Laboratories (LPARL) by J.A. DeRuntz, C.A. Felippa, T.L. Geers and K.C. Park. These three groups targeted different applications and pursued different problem-decomposition techniques. For example, Belytschko and Mullen [9–11] studied node-by-node partitions and subcycling whereas Hughes, Liu and coworkers developed element-by-element implicit–explicit partitions [12–14]. The latter work evolved at Stanford into element-by-element iterative solvers [15]. The work of these two groups focused on structure–structure and fluid–structure interaction treated by all-FEM discretizations.

The remainder of this section (and article) focuses on the authors' work. Research in Coupled Problems at LPARL originated in the simulation of the elastoacoustic underwater shock problem for the Navy. In this work a finite element computational model of the submerged structure was coupled to Geers' Doubly

Asymptotic Approximation (DAA) boundary-element model of the exterior acoustic fluid [16–19]. In 1975 a staggered solution procedure, used in Section 5 as case study, was developed for this coupling. This was presented in a 1977 article [8] and later extended to more general applications [20,21]. The staggered solution scheme was eventually subsumed in the more general class of *partitioned methods* [22,23]. These were surveyed in several articles during the 1980s [1,24,25].

In 1985–86 Geers, Park and Felippa moved from LPARL to the University of Colorado at Boulder. Park and Felippa began formation of the Center for Aerospace Structures or CAS (originally named the Center for Space Structures and Control). Research work in coupled problems continued at CAS but along individual interests. Park began work in computational control–structure interaction [26,27], whereas Felippa began studies in superconducting electrothermomagnetics [28]. Charbel Farhat, who joined CAS in 1987, began research in computational thermoelasticity [29] and aeroelasticity [30]. The latter effort prospered as it eventually acquired a parallel-computing flavor and was combined with advances in the FETI parallel structural solver [31,32].

Research in Coupled Problems at CAS was given a boost in 1992 when the National Science Foundation announced grantees for the first round of Grand Challenge Applications (GCA) Awards. This competition was part of the US High Performance Computing and Communications (HPCC) Initiative established in 1991. An application problem is labeled a GCA if the computational demands for realistic simulations go far beyond the capacity of present sequential or parallel supercomputers. The GCA coupled problems addressed by the award were: aeroelasticity of a complete aircraft, distributed control–structure interaction, and electrothermomechanics with phase changes.

A renewal project to address multiphysics problems was awarded in 1997. This grant addresses application problems involving fluid–thermal–structural interaction in high temperature components, turbulence models, piezoelectric and control-surface control of aeroelastic systems, and optimization of coupled systems. These focus applications are interweaved with research in computer sciences, applied mathematics and computational mechanics.

5. Acoustic fluid–structure interaction

5.1. The source problem

The original coupled problem that motivated the development of partitioned analysis procedures for coupled systems is depicted in Fig. 9(a). A linear or nonlinear three-dimensional structure, externally fabricated as a stiffened shell, is submerged in an infinite compressible fluid (water). A pressure shock wave propagates through the fluid and impinges on the structure. Because of the fast nature of the transient response, which spans only milliseconds, the fluid can be modeled as an acoustic medium.

As shown in Fig. 9(b) the structure is discretized by finite element methods. For the fluid, a boundary-element method (BEM) discretization is convenient as only a surface mesh has to be created. These modeling decisions were dictated by the fact that the structure response (especially as regards survivability) is of primary concern whereas what happens in the fluid is of little interest. The fluid was modeled by the first-order Doubly Asymptotic Approximation (DAA_1) of Geers [16,17] which allowed the replacement of the exterior fluid by its wet surface. This "DAA_1 membrane" is asymptotically exact in the limits of high and low frequencies, hence its name.

Fig. 9(c) reinforces the message that FEM and BEM meshes on the "wet surface" do not generally coincide: one fluid element generally overlaps several structural elements. This happens because stress computation requirements generally demand a finer structural discretization, whereas the main function of the fluid elements is to transmit appropriate pressure forces.

The semi-discrete governing equations for a linear structure interacting with an DAA_1 exterior-fluid model – after some computational rearrangements for the latter – are

$$\mathbf{M}_s\ddot{\mathbf{u}} + \mathbf{D}_s\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}_s - \mathbf{T}\mathbf{A}(\mathbf{p}^I + \mathbf{p}), \quad \mathbf{A}_f\dot{\mathbf{q}} + \rho c\mathbf{A}_f\mathbf{M}_f^{-1}\mathbf{A}_f\mathbf{q} = \rho c\mathbf{A}_f(\mathbf{T}^T\dot{\mathbf{u}} - \mathbf{v}^I). \tag{5}$$

For the structure model: $\mathbf{u} = \mathbf{u}(t)$ is the structural displacement vector, $\mathbf{M}_s$, $\mathbf{D}_s$ and $\mathbf{K}_s$ the structural mass, damping and stiffness matrices, respectively, and $\mathbf{f}_s$ collect forces directly applied to the structure. For the

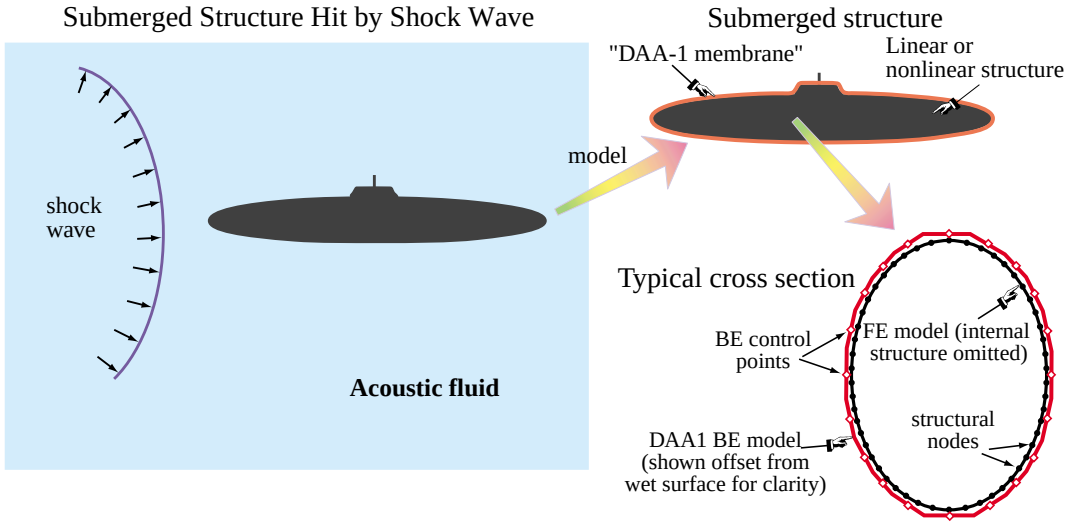

Fig. 9. Submerged structure hit by shock wave: (a) physics of the coupled system, (b) acoustic fluid modeled as "DAA_1 membrane", (c) typical cross-section of coupled FEM-BEM discretization on the wet surface with the interior structure omitted. In (b) and (c) the BEM fluid model is shown offset from the structure for clarity.

fluid model: $\mathbf{M}_f$ is the full, symmetric fluid mass matrix, $\mathbf{A}_f = \mathbf{A}_f^T$ the diagonal matrix of fluid-element areas, $\mathbf{v}^I$ the vector of incident normal-fluid-particle velocities $\mathbf{p}$ and $\mathbf{p}^I$ are the scattered and incident components, respectively, of the nodal pressure vector, and vector $\mathbf{q} = \dot{\mathbf{p}}$ is defined for convenience. All fluid matrices and vectors are referred to the control points of the wet-surface BEM mesh. The two meshes are related by $\mathbf{T}$, which is the transformation matrix that relates node forces at wet-surface structural nodes to fluid-control-point node forces. This matrix is completed with zero rows for internal structural freedoms.

5.2. Two-field FSI: staggered solution

Initial studies using the coupled system (5) dealt with its validation against experiments conducted by the Navy in 1973 on a submerged ring-stiffened cylindrical shell; later known as "the ONR shell" in the underwater shock community. (Test results have been recently freed of publication restrictions.) The simple axisymmetric models used for this testbed permitted experimentation with both field elimination and monolithic solution techniques. Experimental validation (Fig. 10) showed that the DAA_1 and interaction model adequately captured the peak-velocity physics.

The next step was challenging: to incorporate this analysis capability into a 3D production code. The development of a new large-scale structural program was ruled out because Navy contractors were already committed to existing FEM codes such as NASTRAN and GENSAM. (Over the next two decades, ADINA, STAGS and DYNA3D were added to the list.) Implementing a monolithic solution with a commercial code such as NASTRAN, however, rans into serious logistic problems. First, access to the source code is difficult if not impossible. Second, even if the vendor can be persuaded to create a custom version to be used in classified work, upgrading that version to keep up with changes in the mainstream product can become a contractual nightmare.

The staggered solution approach circumvented that logistic difficulty. A three-dimensional BEM fluid analysis program called USA (for Underwater Shock Analysis) was written and data coupled to several existing structural analysis codes over the years, as sketched in Fig. 11(a). For example, the marriage of USA and NASTRAN is called USA-NASTRAN. This plug-in modularity has important advantages. It simplifies upgrade and maintenance of the more complex part, which in this problem is the structural analyzer. Furthermore the latter can be "plug replaced" to either fit existing structural models or the problem at hand. For instance, if the structure experiences strong nonlinear material behavior, the well tested material library, contact algorithms, and highly efficient explicit time integration capabilities of DYNA3D may be exploited.

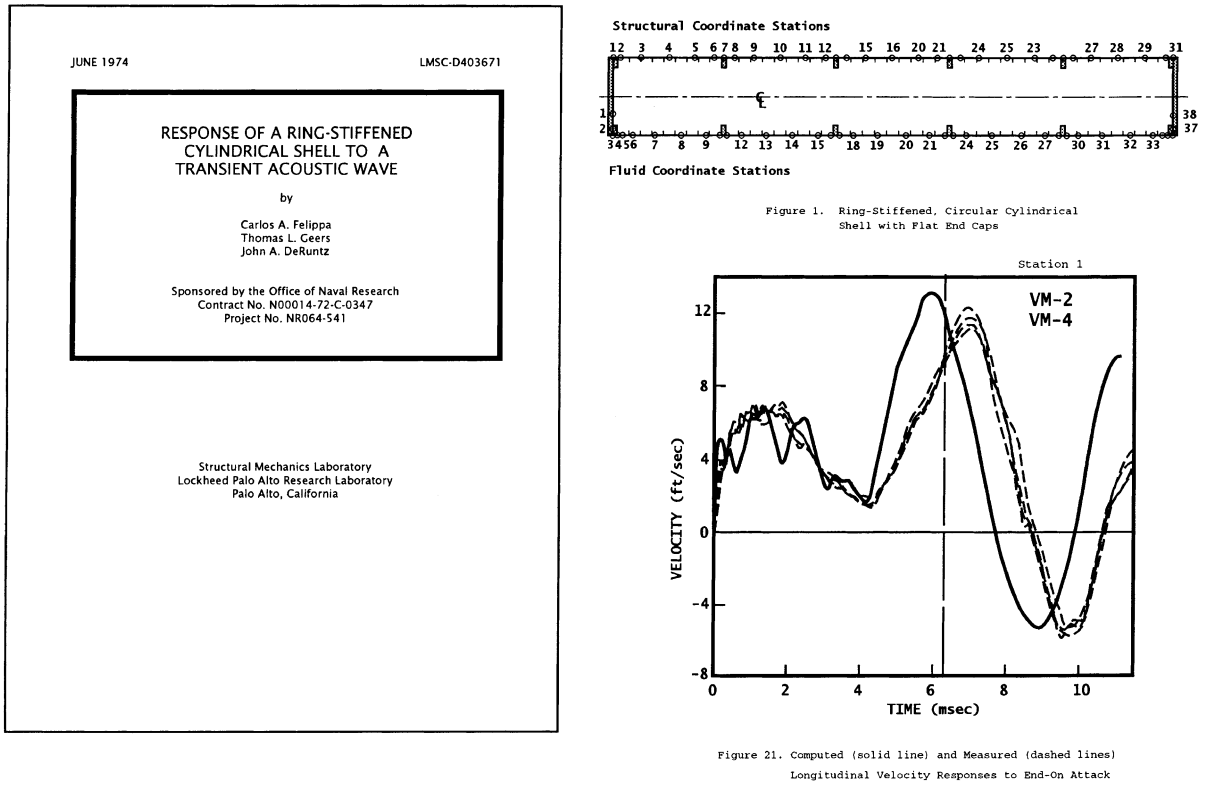

Fig. 10. Validation of the structure-DAA$_1$ fluid model by underwater shock experiments. (Extracted from the original report.) Despite the crudeness of the axisymmetric FSI model shown on top right, most of the important peak velocities, e.g., at shell caps upon end-on attack (lower right), were surprisingly close. This FSI model was eventually adopted to assess vulnerability of actual structures to underwater shock.

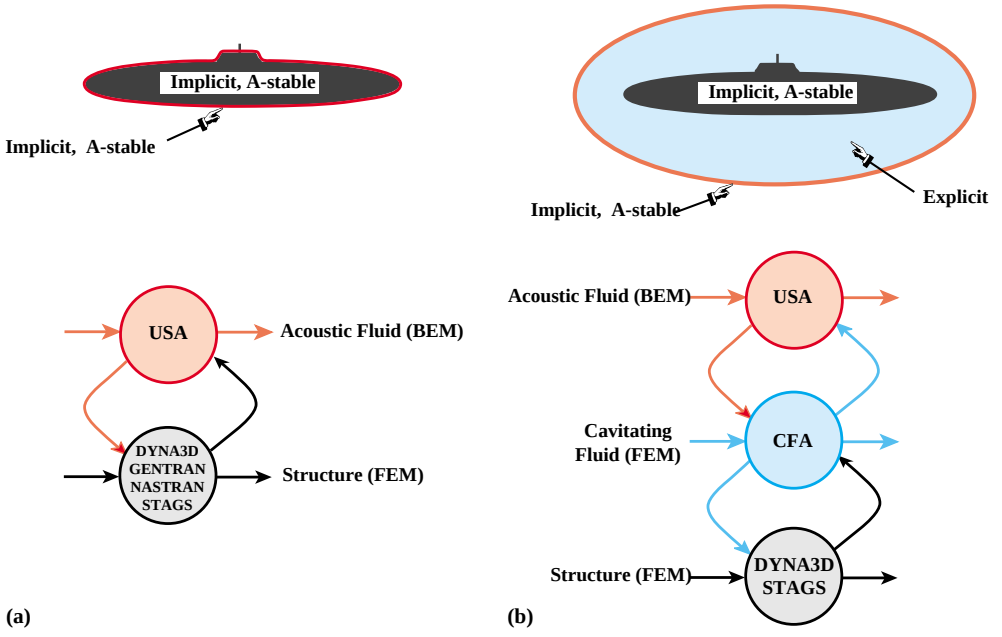

Fig. 11. Implementation of partitioned analysis treatment of underwater shock analysis: (a) as two-field problem coupling acoustic fluid and submerged structure models, (b) as three-field problem coupling acoustic fluid, cavitating fluid and submerged structure models.

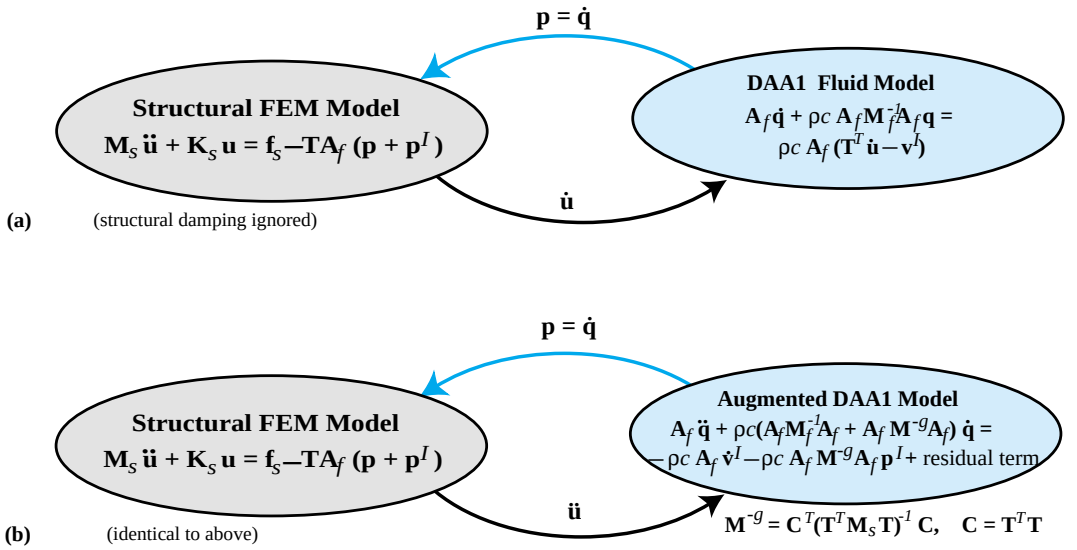

Fig. 12. Reformulation of two-field semidiscrete FSI equations: (a) original (after some DAA_1 rearrangements), (b) upon augmentation of fluid model by structural terms. Augmentation permitted A-stability to be retained in staggered solution.

An additional advantage is computational efficiency per time step. Let us assume that implicit time integration is used on both systems. The structural system is large but sparse whereas the fluid system is dense (because $\mathbf{M}_f$ is full) but small. A monolithic marriage produces a large system where sparseness is severely hindered by the fluid coupling. In the staggered approach the cost per step is roughly the same as that of processing the FE and BE models as separate entities. For realistic 3D structures the cost is dominated by that of solving the structural problem. The overhead introduced by the flow of information is insignificant because it consists exclusively of computational vectors of dimension equal to the number of BEM control points on the wet surface.

If this sounds too good to be true, it is. The high computational efficiency per time step is counteracted by the fact that satisfactory numerical stability is hard to achieve. In fact the practical feasibility of the staggered approach hinged entirely on the stability analysis. In the original publication [8] it is shown that maintaining A-stability for this problem requires a *reformulation* of the governing equations. This is done by a procedure called *augmentation* [1,8,21], which involves transferring selected properties of the structure to the fluid model. The result is that the semidiscrete DAA_1 model is modified as sketched in Fig. 12. This strategy was considered preferable to augmentation of the structural model, because the structural analysis program, for the reasons noted above, was deemed to be untouchable.

5.3. Three-field FSI: cavitation

A BEM treatment of the acoustic fluid works well as long as the fluid is linear. But if the shock wave is strong and the ambient hydrostatic pressure small, bulk cavitation may occur. If the structure is sufficiently flexible, hull cavitation may occur. In either case the fluid must be modeled as a *bilinear* acoustic fluid, and a BEM treatment for the volume affected by cavitation is not possible. It is then convenient to partition the coupled system into 3-fields, as sketched in Fig. 11(b). The near-field, where cavitation takes place, is modeled by acoustic fluid-volume elements. This region is truncated by a DAA_1 boundary. This is an example of a partition driven by local physics.

Accordingly, cavitation analysis was implemented as the three-field coupled system diagrammed in Fig. 11(b). A second fluid program, called CFA (for Cavitating Fluid Analyzer) was written and data coupled to the other two. Thus USA-CFA-STAGS, for example, denotes the linkage of USA and CFA with the nonlinear structural analysis program STAGS. The structure, near-field fluid volume and DAA boundary were processed by implicit, explicit and implicit time-stepping, respectively. It is important to

note that the state of the explicit partition must be evaluated and advanced at half time stations $t_{n+1/2}$, whereas implicit partitions are processed at full time stations t_n and t_{n+1}. With this and other precautions the stable timestep, which is controlled by the CFL condition in the cavitating fluid mesh, was not degraded [21].

6. Beyond shocks

Since the source problem described above, partitioned methods have been applied by us and other research groups to the simulation of coupled problems in structure–structure interaction, thermomechanics, control–structure interaction, and various kinds of fluid–structure interaction involving fluid flow for aeroelasticity as well as in porous media. Because of space limitations the following outline is necessarily sketchy. It is restricted to applications treated by the authors, or deemed to hold future interest.

6.1. Aeroelasticity

The application of partitioned methods to exterior aeroelasticity was pioneered by Farhat and coworkers since 1990 [30,33–39]. The long ambitious long term goal of this project is *to fly and maneuver a flexible airplane on a massively parallel computer*. The essential physics involves the interaction of an external gas flow described by the Navier–Stokes equations, with a flexible aircraft, as illustrated in Fig. 13(a). The aircraft structure is modeled by standard shell and beam finite elements and is advanced in time by an A-stable integrator such as the midpoint rule. The fluid is modeled by fluid volume elements that form an unstructured mesh of tetrahedra and is advanced in time by Runge–Kutta methods. Additional algorithmic and modeling details are provided in recent publications [36–39].

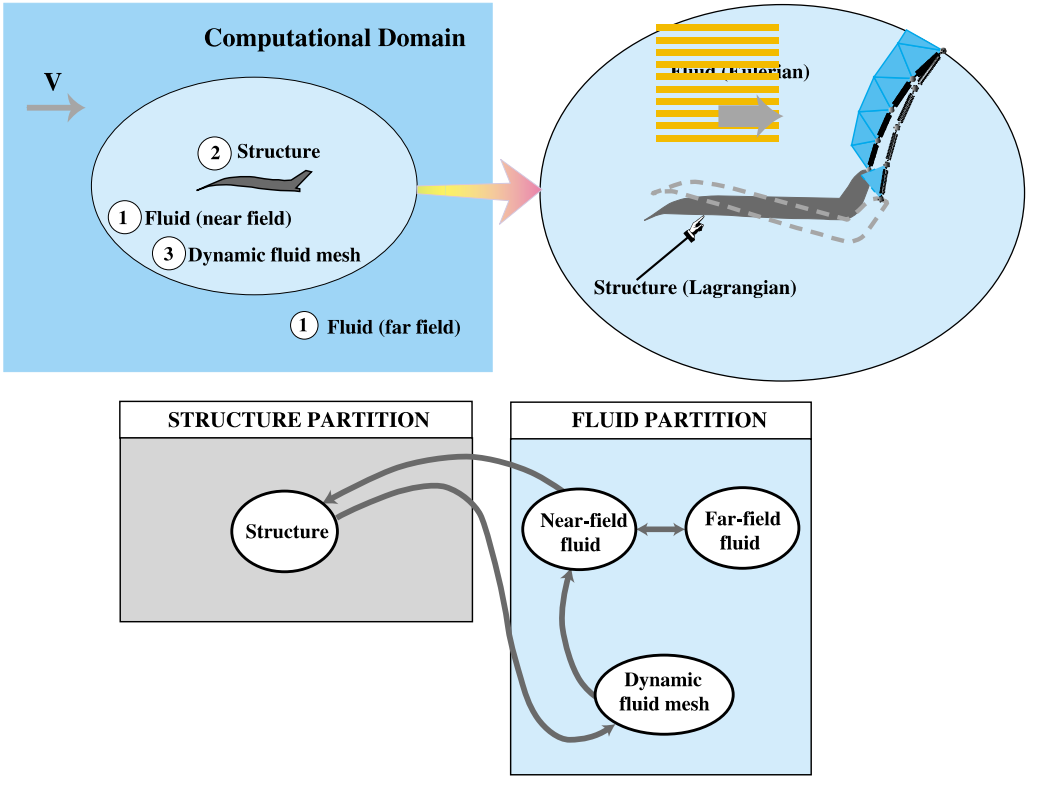

Fig. 13. The exterior aeroelastic problem as a three-field, two partition system.

Three complicating factors appear in this application: *parallel computation*, the *ALE* (Adaptive Lagrangian–Eulerian) *treatment*, and different *response scales*. The influence of parallelism is discussed in Section 6.5. The second complication arises because the structure motions are described in a Lagrangian system, in which the structural mesh follows its motion, whereas fluid flow is described in a Eulerian system, in which the gas passes through the fluid mesh. Hence the fluid mesh, or at least a near-field portion of it, must displace in lockstep with the structural motions.

There are many proposed ALE solutions that work well in two dimensions, but which often lose robustness in three dimensions because of mesh cell collapse. The approach selected in this project exploits an idea originally proposed by Batina [40]. A fictitious network of linear springs, which may be augmented by dampers and torsional springs, is laid down along the edges of the fluid volume elements, as sketched in Fig.13(b). This network may be viewed as a coupled computational field embedded within the fluid partition. The springs are fixed at the outer edges of the region where ALE effects are deemed important. They are driven by the motion of the aircraft surface, and operate as transducers that feed this motion, appropriately decaying with distance, to the fluid mesh nodes. The motion of the dynamic mesh must satisfy geometric conservation laws [37]. The resulting three-field interaction is diagramed in Fig. 13. Although the diagram is topologically similar to the three-field cavitating FSI of Fig. 11(b), the nature of flow computations makes this a more challenging problem.

In commercial aircraft aeroelasticity, structural motions are typically dominated by low frequency vibration modes. On the other hand, the fluid response must be captured in a smaller time scale because of non-stationary effects involving shocks, vortices, and turbulence. Thus the use of a smaller timestep for the fluid is natural. This device is called *subcycling*. The ratio of structural to fluid timesteps may range from 10:1 through as high as 1000:1, depending on problem characteristics and the use of explicit or implicit fluid solver.

6.2. Control–structure interaction

Partitioned solution methods have been also applied to the problem of interaction of an active control system with a "dry" structure; that is, a structure not coupled with a fluid [26,27,41,42]. The interaction diagram for this two-field problem is shown in Fig. 14(a). One novelty is the modeling of the control partition as a second-order system, which permits stabilization techniques previously studied for structure–structure interaction [22,23] to be used as starting point.

The interaction of a control system with a "wet" structure (a structure that interacts with a fluid flow) is a more formidable problem which is the presently the subject of active research. Fig. 14(b) shows the diagram of this three-field coupled system. Envisioned applications include piezoelectric flutter and

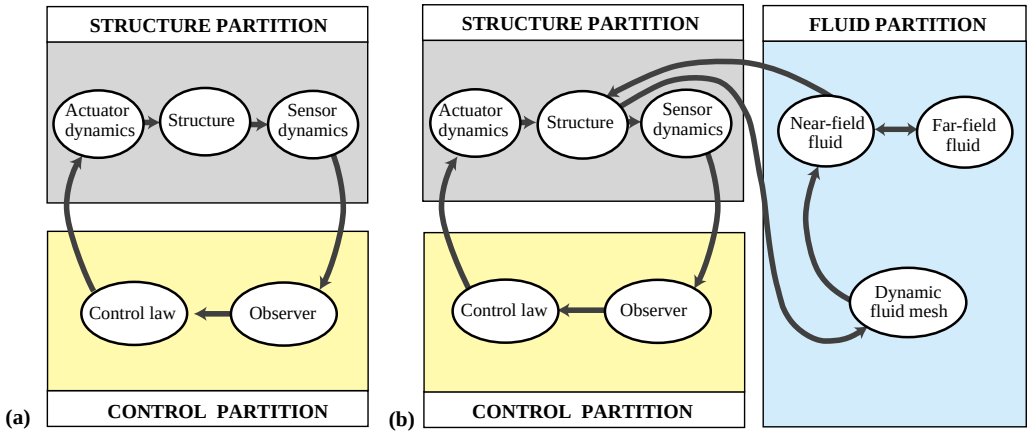

Fig. 14. Active control of dry and wet structures as: (a) two-field, (b) three-field coupled systems.

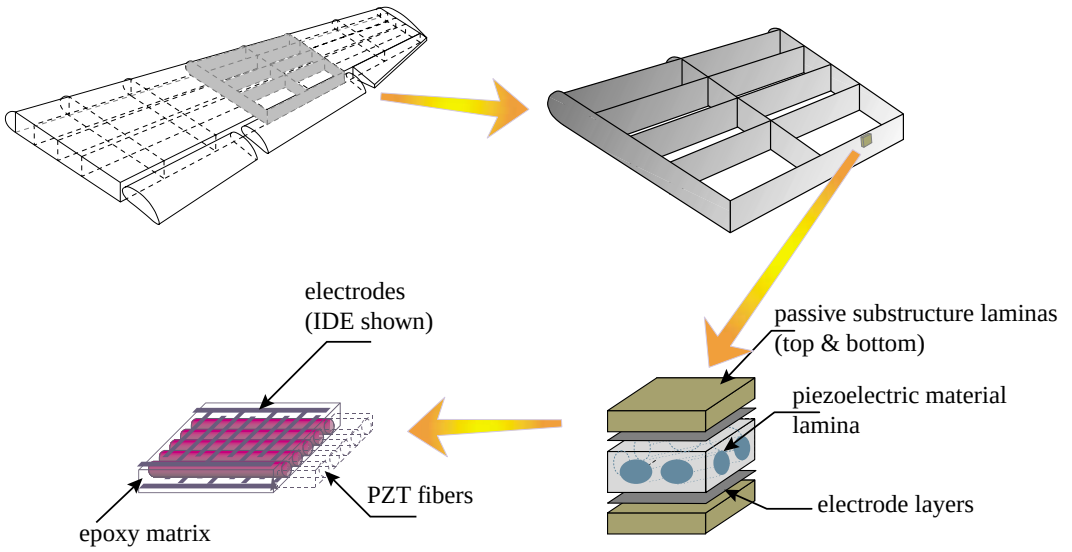

Fig. 15. Piezoelectric control of wing shape for vibration and flutter suppression.

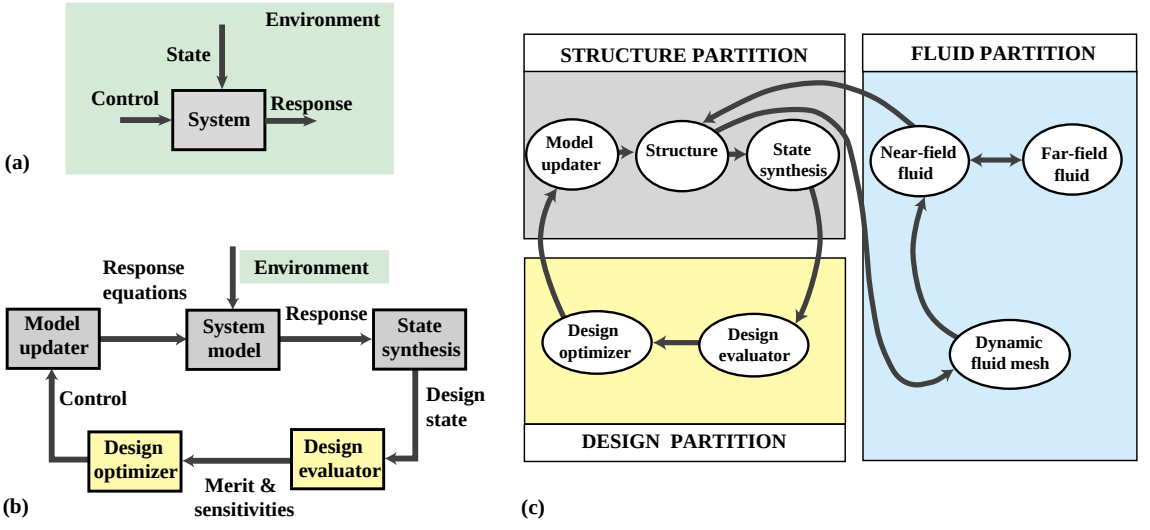

Fig. 16. Computer driven design and optimization of a wet structure as component of a coupled system: (a) abstract interpretation as optimal control problem, (b) practical computer implementation, (c) partitioned analysis diagram.

vibration suppression in aircraft wings, as diagramed in Fig. 15, and stall flutter reduction in helicopter blades [43,44].

6.3. Design and optimization as coupled system

Computer-driven optimization may be embedded in a partitioned framework by recasting it as a control problem [45,46]. The block-diagram of this interpretation is sketched in Fig. 16(a), and a practical realization shown in Fig. 16(b). A design driver program outputs control variables that modify the system model. This model, subject to environmental interactions (for example, with a surrounding fluid) produces a response from which state variables are synthesized and fed to the design evaluator, which supplies design merit and sensitivities to the optimizer to close the loop.

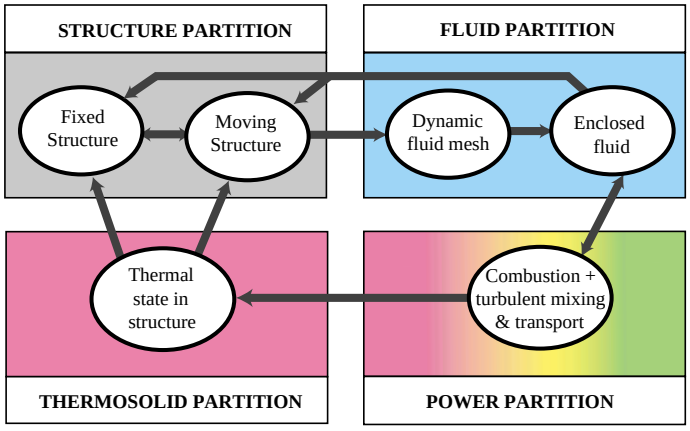

Fig. 17. Simulation of a high-temperature gas turbine engine as four-field coupled system.

The block diagram of Fig. 16(b) formally looks like the control partition of Fig. 14(b). It may be – at least in principle – made into a "design partition" of a coupled system. This interpretation suggests a parallel implementation and points the way to future research into simulation-based adaptive design. For example, can we optimize an airplane (or golf ball) as it flies?

6.4. Gas turbine simulation: a four-field coupled system

The simulation of a high-temperature gas turbine (for aircraft, powerplants or micromotor applications) involves the interaction of four partitions shown in Fig. 17: structure (moving and fixed), enclosed fluid flow, power (combustion, turbulence and transport) and heat conduction. This is an ambitious application that presently lies beyond our modeling and computer power. It points the way, however, to the kind of systems that may be treated in the next century as petaflop parallel computers become available.

6.5. Parallelization

The gradual evolution and acceptance of massively parallel computers over the past decade has brought new opportunities as well as challenges to partitioned analysis methods.

The opportunities are obvious. Massive parallelization relies on divide and conquer: breaking down the simulation into concurrent tasks. Since partitioned analysis relies on spatial decomposition, it provides an appropriate top-level start. One may envision, for example, that in a FSI problem a parallel computer is able to advance the fluid and structure states simultaneously.

This picture, however, is a gross oversimplification. First, there is no guarantee that the computational load will be balanced. For example in the DAA_1-structure models discussed in Section 5 the structure dominates the computational effort, whereas the opposite is true in aeroelasticity. Second, existing parallel computers have more than two processors: typically 16–512 in commercial systems. Thousands of processors are available in the custom, fine-grained parallel machines installed or under procurement at several Department of Energy laboratories. To take advantage of such fine granularities, it is necessary to introduce additional decomposition levels. These are generically called *subdomains*. The decomposition is done by programs called domain decomposers or mesh decomposers. Unlike coupled field partitions, subdomain decomposition is computationally driven. Subdomains, or sets of subdomains, are then mapped to processors.

A two-level decomposition and CPU-mapping procedure is illustrated in Fig. 18. One result of the partitioned approach is that CPUs are "colored" or tagged according to the program they execute. The figure assumes that for an exterior aeroelastic problem the structure, fluid and dynamic mesh are decomposed into 16, 64 and 25 subdomains, respectively (the restriction to perfect squares is only for visualization convenience). If each subdomain maps to one processor, the simulation will use

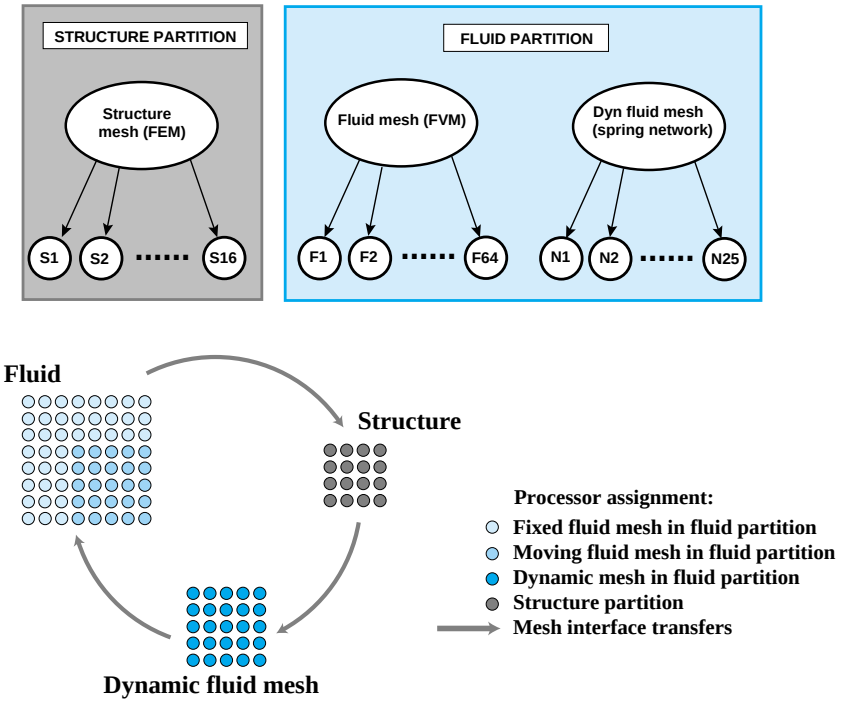

Fig. 18. The top figure shows two decomposition levels in parallel analysis of a coupled system: partitions and subdomains; illustrated for the exterior aeroelastic problem. Bottom figure depicts a one-to-one mapping of subdomains to processors of massively parallel computer. A three-field partition is shown for illustrative purposes only: in present implementations the dynamic mesh is part of the fluid solver.

$16 + 64 + 25 = 105$ processors. Of these, 16 execute the structure code, 64 the fluid code and 25 the ALE code. Each of those processors runs its program copy on different data structures predefined by the domain decomposition. Information transfer between programs is of two types. *Intrapartition transfers* (such as structure to structure or fluid to fluid) are handled by standard message passing techniques based on protocols such as MPI. *Interpartition transfers* (such as structure to fluid or vice-versa) are also handled by messages but may require a mesh interpolation procedure because mesh nodes do not necessarily match at physical interfaces. The time-stepping, sketched in Fig. 19, is carried out using staggered schemes suitably improved and refined for subcycling and computational load balancing.

6.6. Adapting to changes

Since emerging in the mid 1980s, commercial parallel architectures have advanced rapidly, particularly in storage and communications. The flexibility of partitioned methods has facilitated adaptation. Three examples are noted here. On shared memory machines such as SGI's it has been found convenient to allow mapping of several subdomains per CPU, sizing subdomains so each fits in a L2 cache. This generalizes the "one subdomain, one CPU" rule of earlier days. Protocols for processor-to-processor communication are evolving from message passing libraries such as MPI to faster socket connections. Selected programs such as mesh decomposers and visualizers have been recoded in more modern languages, while keeping legacy code in some field analyzers.

Parallel algorithms are also evolving to accommodate architectural advances and experience. Noteworthy developments in the aeroelasticity problem concern *uncollocated staggered algorithms*, in which time stations for fluid and structure may be shifted to exploit the accuracy of midpoint methods while maintaining parallelism through backward corrections. Two improved schemes of this nature for serial and parallel processing are diagrammed in Fig. 20. Technical details are given by Lesoinne and Farhat [39].

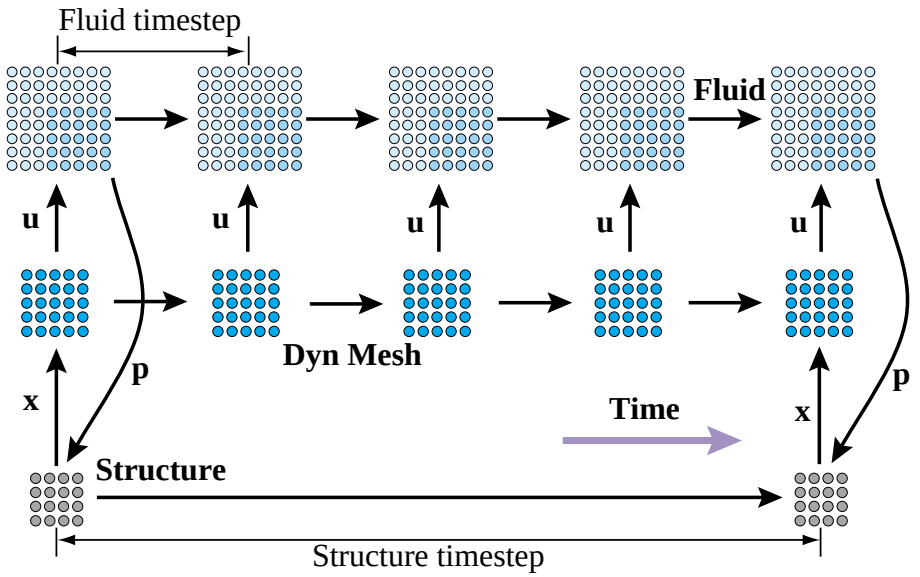

Fig. 19. Parallel time-stepping of the mapping of Fig. 18. This is an idealized diagram prepared in 1993. Adaptation to new architectures and algorithm development have produced variations outlined in the text.

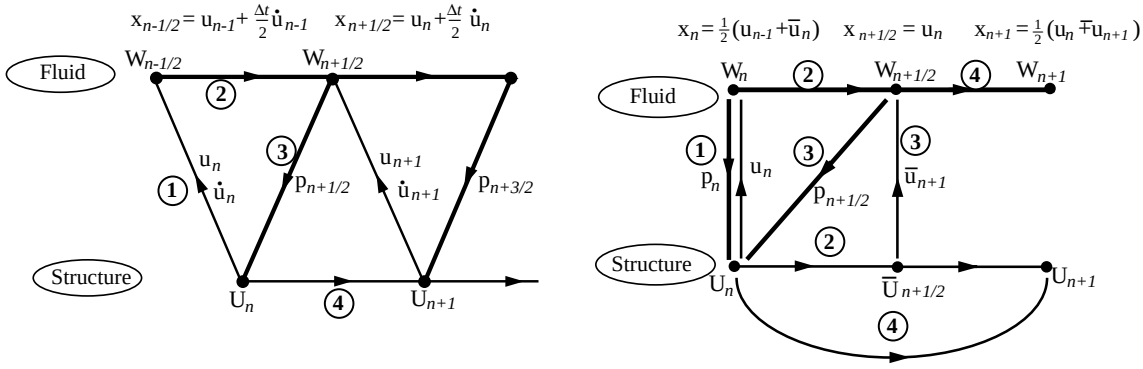

Fig. 20. Improved serial and parallel staggered procedure for the exterior aeroelasticity problem. U and W are the structure and fluid state variables, respectively. From Ref. [39].

6.7. Related work

Several research groups have addressed coupled problems using both monolithic and partitioned schemes. A large portion of the European work during the 1980s is covered in several edited proceedings [47–49]. Staggered procedures have been applied by Schrefler and coworkers to soil consolidation problems with varying degree of success [50–52]. Experience with partitioned schemes at Swansea are surveyed in the second volume of the Zienkiewicz–Taylor monograph [53]. The thesis of Armero [54] is noteworthy for the careful mathematical treatment of dissipative coupled problems using the theory of dynamical systems.

7. Research areas

Some areas that deserve further study in conjunction with the partitioned analysis of coupled systems are listed below.

Stability. This is an important concern. The ideal goal is: *a partitioned treatment should not degrade the numerical stability of the individual subsystems*. More specifically:

1. If each partition is treated by unconditionally stable time-stepping methods, the integration of the overall coupled system should retain unconditional stability.
2. If one or more partitions are treated explicitly and the maximum stable timestep is $h_{\max}$, the integration of the overall system should be stable up to that stepsize.

These goals may be difficult or impossible to achieve without a reformulation (by augmentation) of the original field equations, as in the case study of Section 5.

Stability analysis by standard Fourier techniques using a scalar test equation is not generally possible because modes of individual subsystems are not modes of the coupled problem. For diagonalizable linear models it is possible to use test systems containing as many modes as partitions, as outlined in Appendix A.

Accuracy. In linear problems response tracing accuracy is generally checked only after a stable algorithm is developed. Accuracy degradation is of concern in many applications. A common scenario is: second-order accurate algorithms are used in each subsystem, but the accuracy of the partitioned integration is only first-order. An analysis technique based on the Modified Equation Method is outlined in Appendix A for linear systems. This backward-error analysis, if applicable, provides the global accuracy order directly. A related research area is the study of tradeoffs between interfield iteration versus timestep reduction.

For nonlinear problems stability and accuracy are often interwined and should be studied concurrently. The most promising approach seems to be the use of energy methods applied either to the entire system [36], or to interfield energy exchanges [55]. A general theory of stability of discrete and semidiscrete nonlinear coupled systems remains to be developed.

Interface modeling. This topic has received increased attention with the development of domain decomposition solvers over the past 15 years. These solvers exploit information transfer between matching or non-matching *intrafield* meshes. For example: structure to structure, and fluid to fluid. Much remains to be done, however, for *interfield* non-matching discretizations as well as silent boundaries.

Non-smooth problems. The use of partitioned analysis procedures in applications involving contact and impact merits study to assess whether those methods can provide breakthroughs in modeling and computational power. Related to this topic are problems involving sliding solid and fluid meshes, as in turbomachinery, parachuting, and store separation.

Treatment of volume and non-local couplings. Problems of fluid turbulence, transport and mixing fall into this category, as do applications in metal and plastic forming and thermochemical processes such as combustion. The propagation of non-local effects across partition boundaries can incur significant computational overhead unless clever mesh overlappings or rezoning techniques are developed.

8. Concluding remarks

It is hoped that the present article will give the reader a feel for the largely unexplored subject of coupled system simulation. Even with our stated restriction to mechanical systems of importance in engineering, there remains a great wealth of opportunity for theory, physical modeling, algorithms and simulation. Further multidisciplinary richness pours forth if multiphysics effects are considered. The availability of high performance parallel computers of teraflop power and beyond promises to be a source of exciting theoretical, modeling and algorithmic advances. But any such development must necessarily be subjected to the ultimate test of experimental validation.

Acknowledgements

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Appendix A. Spectral techniques for stability and accuracy analysis

It is well known that the analysis of stability and accuracy of time integration schemes for linear, semidiscrete, undamped structural dynamics: $\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}(t)$, is reduced to that of a model (test) scalar ODE: $\ddot{x}_i + \omega_i^2 x_i = 0$, where i runs over the free-vibration modes. If that structure is coupled to an acoustic medium modeled by a first-order symmetric BEM, as in problem (5), spectral techniques can be used to obtain a 2-equation coupled model system: $\ddot{x}_i + \omega^2 x_i + a y_i = 0$ and $\xi \dot{y}_j + \mu y_j + b x_j = 0$, where i runs over structural modes and j over fluid-boundary modes [8]. For a linear coupled system with n fields, each satisfying diagonalization conditions, the model system will generally contain n coupled ODEs of generally different orders. As an example, if the components of a 3-field system have 10^6, 10^5 and 10^4 freedoms, respectively, there will be 10^{15} model systems of 3 equations each.

If this reduction is possible a precise analysis of stability and accuracy of partitioned methods can be done using spectral techniques. The methodology offers some novel aspects that are illustrated below for a test system of two coupled first-order ODEs.

A.1. Stability by the Amplification Method

Suppose that the analysis of a semidiscrete system of two coupled first-order ODE systems can be reduced to the model system:

$$\begin{bmatrix} \dot{x} \\ \dot{y} \end{bmatrix} + \begin{bmatrix} a_{xx} & a_{xy} \\ a_{yx} & a_{yy} \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \text{or} \quad \dot{\mathbf{z}} + \mathbf{A}\mathbf{z} = \mathbf{0}. \tag{A.1}$$

Here x and y are modal amplitudes of a generic $\{x_i, y_j\}$ mode pair, while a_{xx} through a_{yy} are constant real coefficients satisfying $a_{xx} > 0$, $a_{yy} > 0$, $\det \mathbf{A} = a_{xx}a_{yy} - a_{xy}a_{yx} > 0$. These conditions insure exponentially decaying solutions, that is, physical stability. Homogeneous equations can be used because non-interaction forces can be ignored in questions of stability and accuracy.

We study the one-step implicit integrator with constant stepsize h: $x_{n+1} = x_n + \alpha h \dot{x}_{n+1} + \beta h \dot{x}_n$, $y_{n+1} = y_n + \alpha h \dot{y}_{n+1} + \beta h \dot{y}_n$, with $\alpha > 0$ and $\beta = 1 - \alpha$. Apply this to (A.1) to eliminate temporal derivatives. The resulting monolithic difference scheme, called the *modal amplification system* or MAS, is

$$\begin{bmatrix} 1 + \alpha h a_{xx} & \alpha h a_{xy} \\ \alpha h a_{yx} & 1 + \alpha h a_{yy} \end{bmatrix} \begin{bmatrix} x_{n+1} \\ y_{n+1} \end{bmatrix} = \begin{bmatrix} 1 - \beta h a_{xx} & -\beta h a_{xy} \\ -\beta h a_{yx} & 1 - \beta h a_{yy} \end{bmatrix} \begin{bmatrix} x_n \\ y_n \end{bmatrix}, \quad \text{or} \quad \mathbf{B}_m \mathbf{z}_{n+1} = \mathbf{C}_m \mathbf{z}_n. \tag{A.2}$$

The stability of (A.2) can be studied through standard techniques. Set $\mathbf{z}_{n+1} = \lambda \mathbf{z}_n$, where λ is a (generally complex) amplification factor, expand the homogeneous system determinant as a quadratic polynomial in λ, and transform to a Routh polynomial $C_0 + C_1 s + C_2 s^2$ through the involutory mapping $\lambda = (s+1)/(s-1)$. The time-stepping scheme is A-stable if the coefficients $\{C_0, C_1, C_2\}$ are non-negative for any $h > 0$ and all combinations of $\{a_{xx}, a_{yy}, a_{xy}, a_{yx}\}$ that make $\mathbf{A}$ positive definite. This analysis leads to the well-known condition $\alpha \geqslant 1/2$.

On the other hand, treating (A.1) by an x-staggered integrator with predictor $y_{n+1}^{\mathrm{P}} = y_n + \gamma \dot{y}_n$, in which $\gamma \geqslant 0$, leads to a differential-difference MAS:

$$\begin{bmatrix} 1 + \alpha h a_{xx} & 0 \\ \alpha h a_{yx} & 1 + \alpha h a_{yy} \end{bmatrix} \begin{bmatrix} x_{n+1} \\ y_{n+1} \end{bmatrix} = \begin{bmatrix} 1 + \beta h a_{xx} & -\beta h a_{xy} \\ -\beta h a_{yx} & 1 - \beta h a_{yy} \end{bmatrix} \begin{bmatrix} x_n \\ y_n \end{bmatrix} + \begin{bmatrix} 0 & \alpha\gamma h^2 a_{xy} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{x}_n \\ \dot{y}_n \end{bmatrix} \tag{A.3}$$

or $\mathbf{B}_s \dot{\mathbf{z}} = \mathbf{C}_s \mathbf{z}$. If $\gamma \neq 0$, $\dot{y}_n$ comes in through the predictor. This situation is typical of partitioned procedures. It leads to the question: how is the derivative $\dot{y}_n$ computed? This decision pertains to the topic of *computational paths*, initially studied in the context of structural dynamics integration schemes [56]. For such second-order ODEs there are four choices. For first-order ODEs there are only two:

Path 0: Compute from the differential equation (A.1): $\dot{y}_n = -a_{yy} y_n - a_{yx} x_n$.

Path 1: Compute from the difference equation (A.2): $\dot{y}_n = (y_n - y_{n-1} - \beta h \dot{y}_{n-1})/(\alpha h)$.

For the Path 0 choice, (A.3) reduces to

$$\begin{bmatrix} 1+\alpha h a_{xx} & 0 \\ \alpha h a_{yx} & 1+\alpha h a_{yy} \end{bmatrix} \begin{bmatrix} x_{n+1} \\ y_{n+1} \end{bmatrix} = \begin{bmatrix} 1-\beta h a_{xx}+\alpha\gamma h^2 a_{xy}a_{yx} & -h a_{xy}+\alpha\gamma h^2 a_{yy}a_{xy} \\ -\beta h a_{yx} & 1-\beta h a_{yy} \end{bmatrix} \begin{bmatrix} x_n \\ y_n \end{bmatrix}, \tag{A.4}$$

or $\mathbf{B}_s^0 \mathbf{z}_{n+1} = \mathbf{C}_s^0 \mathbf{z}_n$. This is a standard form MAS. The amplification analysis then leads to the A-stability conditions

$$\alpha \geqslant \frac{1}{2}, \quad 1 \geqslant \gamma \geqslant 1-2\alpha. \tag{A.5}$$

For example, the Trapezoidal Rule: $\alpha = 1/2$, is A-stable if γ is in the range $[0,1]$. The analysis of Path 1 is more elaborate because it couples previous solutions, and operational methods must be used [1]. The novel feature of partitioned schemes is that *stability may depend on the computational path*. On the other hand, such dependence disappears in the monolitic scheme (A.2).

A.2. Accuracy by the modified equation method

The accuracy of monolithic schemes is normally studied by standard truncation error analysis. This approach, however, conveys little information as regards the physical model in questions such as dissipativity or dispersion, or whether rigid body motions are preserved.

More insight can be obtained with the Modified Equation Method, also called the Limit Differential Equation Method in previous accuracy studies [1,23]. This approach fits the spirit of backward error analysis: find a system of differential equations, called the *modified system*, which would be exactly sampled by the time-stepping difference system. This system of course depends on the stepsize h. If the difference between the modified and original ODE is, say, $O(h^p)$ then the integration scheme is globally p-order accurate [57]. Furthermore the differences can be traced to specific matrices such as mass, damping and stiffness, and directly compared to physical uncertainties.

Although the Modified Equation Method was introduced over 20 years ago [58], it has not received much attention. A recent revival has been prompted by growing interest in chaotic dynamical systems, for which forward error analysis is meaningless [59].

For our example problem, a modified ODE can be obtained from the original model ODE (A.1) and a difference scheme generically denoted by $\mathbf{B}_h \mathbf{z}_{n+1} = \mathbf{C}_h \mathbf{z}_n$, as follows. Define $\mathbf{D} = (\mathbf{B}_h^{-1}\mathbf{C}_h - \mathbf{I})/h$, which is a function of h. Formally expand the matrix logarithm: $-\log(\mathbf{I}+\mathbf{D}h) = -\mathbf{D} + (1/2)\mathbf{D}h - (1/3)\mathbf{D}h^2 + \cdots$ in ascending powers of h: $-\mathbf{A}_0 - \mathbf{A}_1 h - \mathbf{A}_2 h^2 + \cdots$, in which the $\mathbf{A}_i$ are independent of h. The modified ODE is $\mathbf{I}\dot{\mathbf{z}} + (\mathbf{A}_0 + \mathbf{A}_1 h + \mathbf{A}_2 h^2 + \cdots)\mathbf{z} = \mathbf{0}$. The time integrator is consistent if $\mathbf{A}_0 = \mathbf{A}$. It is globally first-order accurate if $\mathbf{A}_0 = \mathbf{A}$ but $\mathbf{A}_1 \neq \mathbf{0}$. It is globally second-order accurate if $\mathbf{A}_0 = \mathbf{A}$, $\mathbf{A}_1 = \mathbf{0}$ and $\mathbf{A}_2 \neq \mathbf{0}$. These matrices are functions of the parameters α and γ as well as the modal coefficients.

Taking $\mathbf{B}_h = \mathbf{B}_m$ and $\mathbf{C}_h = \mathbf{C}_m$ one recovers the well known result that the monolithic scheme (A.2) is second-order accurate if and only if $\alpha = 1/2$, i.e., the Trapezoidal Rule. Taking $\mathbf{B}_h = \mathbf{B}_s^0$ and $\mathbf{C}_h = \mathbf{C}_s^0$ one finds that the Path 0 staggered scheme (A.4) becomes second-order accurate if and only if $\alpha = 1/2$ and $\gamma = 1$, which lie on the boundary of A-stability. To illustrate the resulting forms, if $a_{xx} = a_{yy} = 1$ and $a_{xy} = a_{yx} = \kappa$, the modified ODEs including up to $O(h^2)$ terms are:

$$\begin{aligned} &\text{monolithic:} \quad \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\dot{\mathbf{z}} + \begin{bmatrix} 1 & \kappa \\ \kappa & 1 \end{bmatrix}\mathbf{z} + \frac{h^2}{12}\begin{bmatrix} 1+3\kappa^2 & \kappa(3+\kappa^2) \\ \kappa(3+\kappa^2) & 1+3\kappa^2 \end{bmatrix}\mathbf{z} = \mathbf{0}, \\ &\text{staggered:} \quad \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\dot{\mathbf{z}} + \begin{bmatrix} 1 & \kappa \\ \kappa & 1 \end{bmatrix}\mathbf{z} + \frac{h^2}{12}\begin{bmatrix} 1-3\kappa^2 & 2\kappa^2 \\ \kappa(3+\kappa^2) & 1+3\kappa^2 \end{bmatrix}\mathbf{z} = \mathbf{0}. \end{aligned} \tag{A.6}$$

This shows that the backward-error accuracy is similar except for the a_{xy} term. Numerical experiments show that the two schemes are roughly equivalent in accuracy if the timestep of the staggered scheme is about 30% smaller than that of the monolithic scheme. Because the former displays higher computational efficiency (which can reach into orders of magnitude depending on problem size and sparsity), the staggered approach is obviously superior for this example. As noted in the main text, conclusions favoring one approach over the other are problem dependent.

Many coupled systems, notably those involving fluid-flow/structure interaction, do not meet the linearity and diagonalization assumptions and the foregoing spectral techniques do not apply. As noted in Section 7, the development of analysis techniques targeted to those cases represents a fertile ground for research.

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