COMPUTATIONAL MECHANICS NEEDS STUDY

FINAL REPORT
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Introduction

In order to assess the needs in computational mechanics over the next decade, we formulated a questionnaire and contacted computational mechanics researchers and users in industry, government, and academia. As expected, we found a wide variety of computational mechanics usage and research. This report outlines the activity discussed with those contacts, as well as that in our own organizations. It should be noted that most of the contacts were made before the recent decline of the defense industry. Therefore, areas which are strongly defense-oriented may decrease in relative importance. In order to facilitate updating of this study, names of a few key researchers in each area are included as starting points for future literature surveys. These lists of names are not intended to represent those persons doing the best research in that area, nor are they intended to be comprehensive. They are, as previously stated, offered as starting points for future literature searches.

Overall, there is currently a broad activity in computational mechanics in this country, with the breadth and depth increasing as more sophisticated software and faster computers become more available. The needs and desires of the workers in this field are as diverse as their background and organizational products.

There seems to be some degree of software development in any organization (although the level of activity is highly variable from one organization to another) which has any research component in its mission. It seems, however, that there is considerable use of commercial software in almost all organizations. In most industrial research organizations, it appears that very little actual software development is contracted out, but that most is done in-house, using a mixture of funding sources. Government agencies vary widely in the ratio of in-house to out-house ratio. There is a considerable amount of experimental verification in most, but not all, organizations. Generally, the amount of experimental verification is more than we expected.

Of all the survey contacts, one or two believe that the resources they are allocated are sufficient, but most do not. Some believe they have only half the resources they need. Some see their resource deficits as short-term, while others see it as a trend which will continue or perhaps worsen. The pessimism is stronger in the defense and aerospace industry.

When considering only the nonlinear development efforts, there appears to be an even mix of geometric and material nonlinearity. There is not much particular emphasis in linear analysis unless it is in extension of current analysis capabilities to larger problems. The primary exception is concern about modeling of composites, where proven methodologies have trailed element and computer hardware development.

Most of the people we spoke to use finite element techniques, but there is some finite difference and boundary element work ongoing. There is also some interest in multiple methods. Coupling of finite elements and boundary elements appears to be of high interest, since the two analysis types are complementary.

Analysis types needed:

- structural modeling
  - Possibly through our own backgrounds, the majority of the people we spoke with were most interested in structural mechanics. Their interest span a wide range of application areas, with some primarily interested in methods, and then providing these methods to other parts of their corporation. There are obviously others who are only interested in using the tools.

- modeling of composites
  - This was a topic that came up over and over, again possibly due to our own interests and knowledge of who to talk to. The expressed interests in the area of modeling composite materials can be broken down as follows:
    - failure modeling of composites
      -- This was an often-expressed interest. It appears to be the consensus that there are not adequate failure models for composite materials, at the ply level. Nobody appears confident that the "smeared" models such as Tsai-Hill will give realistic failure loads or modes when used in conjunction with very detailed (possibly 3-D) models of composite laminates. There is considerable use of multi-mode criteria at the ply level, in which different failure modes are checked to see if failure has occurred. These criteria seem to satisfy the belief of researchers that failure mode is very important in prediction. Names to use in beginning literature searches include L. J. Hart-Smith, K. L. Reifsnider, F. K. Chang.
      -- Progressive failure of composites was an even stronger area of interest. Composite structures are being used more in primary structure, which need to be designed for post-initial-failure performance. Even if first failure can be predicted accurately, there appear to be no generally available progressive composite failure models which are trusted. There is research ongoing in this area in many organizations. Names to use in beginning literature searches include F. K. Chang, C. T. Sun.
    - modeling of textile composites
      -- The desire to use composite materials based on textile preforms, processed by RTM or some other infiltration process, is definitely increasing. There is, however, no accepted modeling technique for prediction of strength, stiffness, etc., of these materials. The reason for the current level of interest in these materials appears to be the belief that they represent cost-effective materials with superior through-the-thickness properties, relative to laminates. Names to use in beginning literature searches include F. K. Koh, C. M. Pastore, T. W. Chou, J. D. Whitcomb, T. Ishikawa, R. L. Foye, I. S. Raju.
      -- It also appears that textile composites may have considerable energy absorbing capability when loaded in compression. Analysis of this, however, requires the ability to model accurately the internal details of the material and conduct a progressive failure analysis at the micromechanics level. It is generally accepted that progressive failure models are required before energy absorption can be computed. Names to use in beginning literature searches include G. L. Farley, H. D. Carden, J. Morton, C. T. Sun.
    - design allowables for composites
      -- There is a tendency for engineers and designers to want to revert to the design philosophies and techniques which were popular for isotropic materials. The concept of design allowables may fall into this category, or it may be that this is just another way of asking for reliable failure theories. It is my personal philosophy that things like design curves are to be avoided, since they may give the impression that composites design is straightforward, which it is not. Also, the existence of such design curves may lead designers to NOT look for revolutionary design concepts, but rather to repeat or scale previously acceptable concepts. Names to use in beginning literature searches include Z. G ürdal , R. T. Haftka, C. C. Chamis.

- life prediction of composite structures
    - -- The definition of "life" of a composite or a composite structure is so nebulous that I don't know what to say about this one. "Durability" may be a synonym for life, and I don't know what to say about that either. This is, I believe, another request for reliable design allowables, primarily in the area of fatigue. Names to use in beginning literature searches include K. L. Reifsnider.
- free edge stresses
    - -- This is a continuing problem. I thought that we had pretty well done it, but the issue now may be to solve the edge problem for very thick composites (e.g. a 5" composite has about 1000 plies, and if you use two 3-D elements per ply, then you have 2000 elements through the thickness of the laminate. This issue may therefore be related to current hardware limitations and/or to the lack of reliable failure criteria.) Names to use in beginning literature searches include C. T. Herakovich, J. D. Whitcomb, I. S. Raju.
    - -- It also appears that textile composites may exhibit edge effects which are a function of their fiber architecture, thus leading to a much broader set of free edge problems than exists for tape layups. There will undoubtedly be new classes of problems for textiles with woven and/or braided edges which behave quite differently than for laminates. There is very little existing literature on this topic.
- analysis of ply drops
    - -- There is a lot of work going on here, and the issue(s) may be the same as for the free edge problem. Certainly ply drops will continue to be a problem as long as we laminate composites, whether the layers are themselves unidirectional tape or possibly a complex textile. There may be analogous problems with weaves and braids. Names to use in beginning literature searches include E. R. Johnson, J. H. Starnes, Jr.
- impact loading of composites
    - -- This issue is relevant to all applications of composites, whether it be spacecraft, aircraft, automobiles, submarines, and so on. It also relates to the ability to run transient analysis of huge problems, and to the reliability of failure criteria, except now there may be rate dependence. This issue is also complicated by the possibility of complex fiber architectures. Names to use in beginning literature searches include J. Morton, G. S. Springer, W. B. Avery, C. T. Sun.
- modeling very thick (5") composites (determine hot spots, auto refinement, 2-D to 3-D, data interpretation)
    - -- Again, this may be a problem of how to run huge models. Global/local methods are definitely an issue, as well as how to extract 3-D information from 2-D models. There are some techniques for this, but they have not been proven yet. I believe the data interpretation aspect here is just another plea for more capable scientific visual analysis capabilities. Names to use in beginning literature searches include J. Fish, J. Ransom, O. H. Griffin, Jr., C. E. Knight, J. N. Reddy, N. J. Pagano.
    - -- This need may decrease with the recent changes in the world situations and apparent decreased need for composite submarine hulls.
- fluid-structure interaction
    - The interest here comes from both aircraft and underwater people. There is interest, quite a bit of it, in coupled aeroelasticity. The Navy people who are working on composite submarines are obviously interested for a number of reasons.

- There are quite a few loading cases of interest here, including shock interaction, which may bring rate dependence into play.
- scientific visual analysis
  - Definitely a hot topic. The interest is driven by advances in graphics, as well as the capability to run 3-D models which are almost impossible to visualize. There are pretty good visual tools there (e.g. PATRAN, AVS), but they leave quite a bit to be desired. Translucency, slicing, and so on will be important in visualizing 3-D information. Multi-media is getting hot in the ability to take computer graphics straight to film and/or videotape. Names to use in beginning literature searches include R. D. Kriz, R. B. Haber.
- contact problems
  - This is driven by a number of things. The interest in contact problems has always been a nasty, but important one. There are a lot of very good gap/contact elements available now, in codes such as ABAQUS. The users are just now finding out how well they work, and are trying to solve some problems that they previously dismissed as intractable. Load proportioning in multifastener mechanical joints is an example. Names to use in beginning literature searches include M. W. Hyer, L. J. Hart-Smith, O. H. Griffin, Jr., J. H. Crews, D. Cohen.
- advanced constitutive models
  - models for stiffness, strength, and life prediction of textile composites Names to use in beginning literature searches include F. K. Koh, T. W. Chou, J. D. Whitcomb, R. L. Foye.
  - advanced plasticity theories, such as the endochronic theory Names to use in beginning literature searches include J. Aboudi, M. J. Pindera, S. Y. Hsu, G. Dvorak, J. Teply, R. A. Schapery.
  - constitutive models which are themselves finite element models, essentially running out of sight of the user. This capability may also be useful in analysis of textile composites. Names to use in beginning literature searches include J. Teply, Y. A. Bahei El Din, S. Y. Hsu.
- want semi-empirical methods
  - My personal opinion is that this goes back to the "design curve," "design allowable" focus. Researchers are being driven (ordered, threatened) that they must deliver tools which can be used by people with very little knowledge in the mechanics of composites to design composite structures.
- reliability analysis
  - This is a multi-faceted area, which deals with analysis of complex loads, geometries, fatigue, failure, and everything else you can think of.
  - Probabilistic methods figure in here, as does the ability to do sensitivity analyses. It appears that at least a portion of this is driven by the need to perform studies of the effects (e.g. load carrying capacity, fatigue life) of known manufacturing inaccuracies in composite structural components. Names to use in beginning literature searches include R. A. Heller, S. P. Englelstad, C. C. Chamis.
- nonlinear/post-buckling
  - It appears that many structures are being designed to operate in post-buckled regimes. Operation in those regimes requires design techniques, analysis capabilities, failure/plasticity modeling, and an array of other capabilities which currently are either nonexistent or too expensive to conduct. Names to use in beginning literature searches include J. Lee, M. P. Nemeth, M. Stein, T. J. R. Hughes, T. Belytschko, G. A. Thurston, M. J. Shuart, J. H. Starnes, Jr.

- At least one person mentioned post-buckling with multiple load cases. This is obviously necessary if one is to design for operation in the postbuckling regime.
- simulation of manufacturing processes and their control
  - This is also bound to be an important topic for many years to come. One of the thrusts, from my viewpoint, appears to be in modeling processing of composite materials. There are considerable heat transfer, mass transfer, fiber bed compaction, and so on, to be modeled. Also, consider the processing of ceramic matrix composites, carbon-carbon, and the other composite materials that are processed at very high temperatures. Near net shape fabrication using processes such as HIP will continue to be of interest. There also appears to be continued interest in superplastic forming. Considerable effort is being directed at various forms of injection molding. Names to use in beginning literature searches include A. C. Loos, G. S. Springer, C. E. Knight, H. B. Dexter.
  - With the recently-demonstrated ability (at IBM, at least) to reorganize materials at the atomic level, we may see the requirement to predict properties and/or processing parameters for materials and/or processing at this level. We did not discover any literature on this topic.
  - Merely analyzing the process is a formidable task. Consider on top of that the desire to control that process in real time. Computational power requirements will be greatly increased.
- smart structures
  - This area will be important for the foreseeable future. The potential of smart structures is just being realized. The number of actuator/sensor combinations is really large. Analysis of the response and control of these structures will be extremely computationally demanding. Once the means to analyze them is available, it will be desirable to have onboard processing so that control can incorporate predicted structural response, or possibly be used for system identification, especially in the presence of damage. Names to use in beginning literature searches include C. A. Rogers, O. H. Griffin, Jr., B. K. Wada, E. F. Crawley.
- crashworthy structures
  - Most crashworthiness concepts have involved addition of parasitic energy absorption devices onto existing structures. It is now time to begin to analyze structural response to crash, and to design crashworthiness into the structure rather than trying to add on energy absorbing devices after the structural design is complete. This inherently requires dynamic, highly nonlinear, contact problem solution, as well as progressive failure analysis. Names to use in beginning literature searches include H. D. Carden, G. L. Farley, C. M. Kindervater, F. Och, R. L. Boitnott, L. Burroughs.
- large angle flapping flexures with follower forces (helicopter blades)
  - Combination of modal analysis, nonlinear analysis (geometry plus follower forces). A very important application as helicopter design becomes more sophisticated. Once they have this capability, they'll want to be able to include fatigue life prediction of composite rotor blades, as well as coupled aeroelasticity. Names to use in beginning literature searches include L. W. Rehfield, T. K. O'Brien.
- biaxial loads at high temperature
  - I believe this is a pretty tricky constitutive problem, which has implications in the ability to develop meaningful test methods to get the constitutive parameters which go beyond the structural analysis implications.

- residual stress modeling
  - In composites, or just about any other material for that matter, this is related to elevated temperature and pressure, and the existence of extremely complicated stress states while at high temperature. The literature is so voluminous and ongoing that picking up any computational or composites journal will yield a starting point for a literature search.
- modeling of manufacturing imperfections
  - This might be a good application of stochastic finite elements. This presupposes the availability of high speed computers capable of running the many required analyses very quickly.
- optimization
  - There is a continuing desire to have optimization as a standard tool for engineering. While in the past optimization has required development of non-finite-element solutions because of the large computer resources required by finite element analysis, it appears to me that FE software (good elements, fast solvers) and computer hardware have come to the point that some optimization may be possible even for complex problems. Given the infinite number of choices available when designing with composites, this capability will, I believe, find wide use. Names to use in beginning literature searches include R. T. Haftka, Z. Gürdal, G. N. Vanderplaats.

Software needs:
- enhanced tools for including effects of delamination in composites
  - This relates to a methods development rather than a basic software issue since the basic mechanics are very poorly understood. Everybody who uses finite elements is still wary of modeling singular problems, and delaminations are really spatially complex singularities, with unknown strengths. A very nasty problem, but a very necessary one to solve if we require solutions to residual strength and/or life in damaged, or merely aging, structures.
- analysis tools that have correct physics and mathematics for composites
  - I agree. There are a lot of patched-up composites elements out there, written by people who don't really understand the mechanics of composites. Perhaps some reliable benchmark problems need to be devised to shake out elements, or even codes, which claim to do composites. Sort of the "composites" version of the MacNeal-Harder cases.
- more design-oriented tools to facilitate rapid parametric studies (materials, layups)
  - Finite elements are notoriously good for analysis, but notoriously bad for parametric studies due to their computational demands and the person-time demands to set them up. The ability to perform parametric studies, especially rapid (wall clock time) parametric studies would be a great thing for practicing engineers. Stochastic finite elements might be applicable in this scenario.
- links to solids modeling/CAD tools
  - This is a continuing problem - how to get information from the design floor into FEA. IGES appeared to be the solution, but I'm not sure any more. There are currently several comprehensive commercial systems which appear to be viable.
- bring state of nonlinear analysis to that of a production tool
  - A nice idea, and one which I'm sure appeals to management everywhere - let the draftsperson do the nonlinear FEA. The requirements for such a thing are considerable. This may require implementation of an expert system to evaluate the solution continuously and alert the "analyst" if something begins to diverge.

- more robust algorithms
  - This is one thing that would have to be done before nonlinear analysis is a production tool. Algorithms and solvers are getting better all the time, but I still get messages that I'd be hard-pressed to explain to someone who didn't have a pretty good background in finite elements and/or numerical analysis.
- marriage of CFD with structural analysis
  - This is obviously something that has to be done eventually so that we can do advanced design, such as for the aircraft of the future. Modular codes such as COMET are the natural place to implement such capabilities.
- multiple methods
  - There was really no stated request for multiple methods, but such formulations appear to me to be necessary in order to perform some of the tasks indicated to be of interest. More direct application of substructuring, elements with built-in singularities of user-selected strength, and single-tool analysis of multi-disciplinary problems where FE is better for one discipline(s) and some other method (e.g. FD, BEM) is better for the other discipline(s) are examples.
- modeling complex situations to reduce testing
  - This will always be a goal. This seems to me to relate back to the ability to control boundary conditions somewhere between the level of "fixed" and "free." Stochastic methods may play a role here, also. The ability to cleanly vary the boundary conditions and determine the effects could lead to better understanding of the mechanics of some very popular tests which often yield results with surprisingly high variability. The complete topic of compressive testing of composite materials falls into this category.
- "adaptive modeling" (I personally like this term.)
  - Included here is the user-oriented implementation of p-, h-p- and other adaptive versions of the finite element method. There are currently several relatively new commercial products (e.g. Mechanica) which offer some of these capabilities.
- quality control
  - Software with built-in error estimation algorithms. This is a great idea. Consider a software package which at the end of the run calculates reliable error estimates of the output quantities.
  - Software which performs checks on the validity of the assumptions made in its own formulation (e.g. checks validity of geometric linearity assumptions based on the computed deflections, rotations, strains, etc.). Software which indicates to the user the maximum loads which can be applied to a structure without inducing material or geometric nonlinearity.
- The ability to analyze general coupled field problems. There are signs of this capability in some commercial packages.
- At the computer system software level, users need object-oriented programming languages, and it should be possible to take this object-oriented approach to the level of structural analysis, especially with modular approaches like COMET.
- User and/or automatic control of inclusion of shear deformation theory.

Training needs:
- how to write optimum code
  - There are still people who don't trust optimizing compilers to write the best code, and people that don't understand that the algorithms must be properly developed or optimum code doesn't help.

- how to write for massively parallel machines
  - This is a basic need, or maybe fear of a need. None of us are sure that we can make the massively parallel machines that are certain to come along soon really hum. Given that we have the algorithms (which is generally not true) if the compilers that go with them can't really parallelize our code, we'll need to learn to do it, at least until the compilers catch up.

Hardware needs:
- faster computers
  - I sincerely doubt that computers will ever be deemed fast enough by most of us. One fellow said, "Now that I have gigaflops, I want teraflops." I think that pretty well sums it up.
- larger memory
  - Same as for speed. There will probably never be computers with quite enough memory.
- more storage
  - Same comment applies.
- advanced backup and user-friendly removable storage devices.
  - models are continuing to grow in size, and advanced graphical approaches are resulting in frequent creation of files of gigabyte size. Users need ready access to removable random access read/write media which can be used for storage and ready recovery of such large files. Serial devices are not generally acceptable, although they are currently the most effective and cost effective means of storing large amounts of data. There are some reasonably large capacity optical drives and "portable" hard drives, but they are not, in general, of sufficient capacity even for current needs. Terabyte devices would be used routinely if available.