Responsible Conduct in Computational Modeling and Research

RCR training for students and professionals

Model development is that act of scientific and/or professional authorship in which salient features of an observable phenomenon are reduced to an accessible formulation that enables the testing of scientific hypotheses in a rigorous and effective manner. As the speed, precision, and display capabilities of computers have increased, computational modeling has become pervasive in engineering and science research and development. This package contains resources for academic instruction and professional training in the responsible conduct of computational modeling and research, providing the reader with a framework within which to establish the integrity and trustworthiness of computational representations and their predictions. The package discusses learning objectives and pedagogical approaches, and provides tools appropriate for use in instruction, including fictional case studies, scoring guides, and check lists.

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Responsible Conduct in Computational Modeling and Research

Resources for academic instruction and professional training through fictional case studies and commentaries, role plays, and tools for formative assessment

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LEARNING OBJECTIVES

INTRODUCTION

Model development is that act of scientific authorship in which salient features of an observable phenomenon are reduced to an accessible formulation that enables the testing of scientific hypotheses in a rigorous and effective manner. The classical engineering sciences have used mathematical models, for example systems of differential equations, that reflect essential properties of a physical system and whose solution describes the system behavior. In the past thirty years, a new class of model development has become feasible, namely, the synthesis of computational models that produce quantitative, numerical information about the behavior of complex systems. Computation extends the analyst's ability to understand the behavior of simple mathematical models for which closed-form solutions may not be available. More importantly, computational modeling and research is now a sub-discipline of existing engineering and science fields. In many cases, researchers can bypass the formulation of a mathematical model and instead reduce system behavior directly to computational algorithms. Examples include research in mechanics that aims to develop computational models to simulate the propagation of a crack in an aluminum plate; research in ecology that models the evolution of plant species in a tropical rain forest; research in solid-state electronics that models the flow of electrons in a compound semiconductor transistor; research in bioengineering that models the mechanics of orthopedic implants; and research in computer engineering that models the execution of instructions in the pipeline of a computer processor.

The responsible conduct of research (RCR) in model development, in general, and computational modeling, in particular, relies on a careful assessment of standards of ethical practice that serve to maintain broad-based trust and reliance on the scientific method in i) the search for testable explanations of natural phenomena, ii) the application of modeling to design and problem solving, and iii) the use of modeling for the formulation of policy recommendations (Kijowski, Dankowicz, & Loui, 2013). The increasing speed, precision, and display capabilities of computers have enabled computational models of complex, high-dimensional phenomena that would not be otherwise amenable to scientific analysis. Trust in the conclusions drawn from such computational modeling relies on maintaining model transparency, reproducibility, and data verifiability. Computational models also challenge principles of authorship, intellectual property, and commercial ownership.

We label here as *ethics* those principles of responsible conduct that promote mutual trust and warrant against misrepresentation. Because scientific research is archival and cumulative, the success of the scientific enterprise depends critically on faithfulness to commonly accepted practices across languages, cultures, and times. Lack of awareness of, or adherence to, mutually accepted principles of responsible conduct among practitioners undermines public trust in scientific principles and raises the specter of capricious policymaking.

At the foundation of the scientific method one finds the modeling paradigm, the search for essentially equivalent, but more manageable representations of observed phenomena. Indeed, it is in the analysis of models that science formulates and challenges hypotheses, develops theoretical frameworks, and draws conclusions about a "reality of interest" (Performance Test Code Committee 60, ASME, 2006). This stage of inquiry is also the least understood by those who rely on subsequent conclusions. There is thus a deep ethical imperative to determine a set of good practices employed in model development and to promulgate these standards of practice widely.

Computational models will continue to provide linkages for interpretation, but as science gets more complex, it can easily become more isolated from nonscientists, whose distrust of science might increase. (Committee on Models in the Regulatory Decision Process, National Research Council, 2007)

OUTCOMES

Whether for class-room instruction or self-study, the identification of instructional objectives and educational outcomes is closely coupled to good teaching and learning strategies that help in the evaluation of material and in the retention of core principles (Kalichman & Plemmons, 2007). For a recent view of the landscape of ethics education, available resources, and the assessment and evaluation of ethics training, we recommend the workshop report *Ethics Education and Scientific and Engineering Research* published by the National Academy of Engineering (Hollander & Arenberg, 2009).

The material in this package aims to enable the reader to:

- Explain the role of trust, transparency and honesty in all scientific endeavors, including computational modeling.
- Recognize responsible conduct issues within computational modeling, including issues related to model integrity, model robustness, model representation, data and code integrity, and intellectual property. Specifically, to
    - Describe the facets required for model integrity, including the agreement of mathematical models with physical phenomena, appropriate computational algorithm choice and implementation, and

verification of code and calculation accuracy through benchmark testing.

  - Identify issues of model robustness, including the effects of error in measured observables.
  - Give examples of how model representation and visualization can be used as powerful tools for making computational modeling accessible, but also how they can be abused and misused.
  - Assess the use of verification of code and calculations, and of experimental validation in responsible computational model development.
  - Characterize the life-cycle of a computational model and the process of revision and version control as it relates to responsible model development.

- Analyze and critique case studies on issues of responsible conduct in computational modeling.
  - Implement case discussion and role-play exercises to create discussion in a classroom setting.
  - Use a decision procedure checklist to assess quality of responses to case studies.

ISSUES AND ACTIONS

INTRODUCTION

It is all too easy in the computational paradigm to compute! Available software implementations perform advanced modeling calculations that produce numerical output even with inconsistent model formulations or data input. Too often great faith is placed in the results of such computations, even when these disagree with fundamental tenets of the underlying theory.

It is incumbent upon the model developer and user to appreciate and adopt generally accepted standards in the formulation of computational implementations and in their dissemination. At the core of this process is an evaluation of the integrity of the model, i.e., i) the degree to which it reflects the phenomenon it purports to study, ii) the degree to which the computational algorithms respect model assumptions, and iii) the degree to which a numerical implementation gives reasonable results while bounding error growth and propagation. The challenge is all the greater in the context of computational models that glue together mathematical formulations at many parallel length and time scales. A proper model evaluation may in such instances lie beyond available tools of analysis.

> *"A good model is one that achieves the right balance between simplicity and complexity to address the question at hand."* (Committee on Models in the Regulatory Decision Process, National Research Council, 2007)

In seeking to capture the salient features of an observed phenomenon, it is necessary to reduce to their core those interactions that influence the phenomenon and to eliminate those interactions that do not. This is clearly a sensitive stage in model development and may make or break any case for policy recommendations or business decisions that might result from subsequent computational analysis. Whereas low-dimensional models that neglect all but one or two contributors to a physical phenomenon may yield valuable insight into critical characte-ristics and qualitative behavior of a complicated system, the utility and validity of complex high-dimensional models are challenging to ascertain. Challenges to model integrity further enter at the stage of implementing computational algorithms in user-friendly software. In addition to obvious concerns related to mistakes in coding logic, numerical software is by necessity restricted to systems with discretely-valued independent variables. Discretization techniques for approximating infinite-dimensional formulations, for example of atmospheric fluid flow, must be chosen with care to prevent the discretization itself from corrupting the computed system behavior.

When possible, computational codes should be accompanied by well-documented benchmark tests, and their predictions preferably tested against experimental observations. For example, computational models of the mechanics of orthopedic implants might be compared to basic experimental studies of implants in cadaveric bones. Computational models of the dynamics of vehicular impacts might be compared to crash test data collected in the laboratory. However, in other circumstances this expectation of experimental validation may not easily be realized; consider, for example, models that seek to predict the risks to human health associated with prolonged exposure to environmental toxins or changes in global climate.

Even where the sensitivity of a model to parameter and input uncertainty raises no concerns for model integrity, researchers must nevertheless qualify their confidence in the reliability of the model's conclusions. This reliability may be problematic when the development involves the reduction of essentially stochastic phenomena to deterministic models.

In experimental contexts, it is common to represent model uncertainty in terms of statistical properties of measured observables, for example error bars that estimate the variance of an associated probability distribution. Similarly, in computational modeling, uncertainty can sometimes be handled through Monte Carlo methods and statistical sampling, sometimes through sensitivity analysis of how changes in the inputs affect the outputs, and sometimes through computation with complex stochastic models. Rather than a weakening of the persuasive power of scientific inquiry, accepted and clearly articulated principles for how to represent and communicate sources of uncertainty and

their influence on model predictions increase public trust in proposed explanations for observed phenomena or subsequent policy recommendations.

To present the results of a simulation, a computational researcher might produce a visualization, for example, an animation of the development of a thunderstorm. Scientific visualizations can look convincing: trial lawyers use visualizations that recreate automobile accidents to persuade juries to accept their interpretations of the events. Because visualizations can be powerful, computational researchers must take special care to create them responsibly.

Visualization affords a powerful means of representing high-dimensional data, for example physical characteristics such as velocity, temperature, density, and pressure in a turbulent fluid flow, or binding energy, kinetic energy, and particle species in a biomolecular reaction. Such simultaneous representations, for example using color intensity for energy and shape for binding energy, may yield substantial insight to the modeler but be misleading if taken out of context. Visualizations may also give an impression of precision where the underlying phenomenon and computational model include significant uncertainties in parameters or inputs. Because visualization has an obvious public-outreach value, awareness of the ethical implications is paramount.

Typical RCR materials advise researchers to record experimental procedures and data with permanent ink on signed and dated pages in bound laboratory notebooks. By contrast, computational researchers keep records in electronic form rather than in lab notebooks because the volume of data is enormous: computer codes can be tens of thousands of lines long; a single simulation run can use 20 gigabytes of input data to produce 50 megabytes of output data—or more.

Ideally, to enable independent verification of the correctness and reproducibility of results and published work, the computational researcher should archive the version of the code and the input data that produced the output data. But because of limits of storage media, it may not be practical to keep every version of the code and every data set. The degree to which computational models may be independently checked is clearly a function of adherence to principles of good coding practice, including code transparency and modularity.

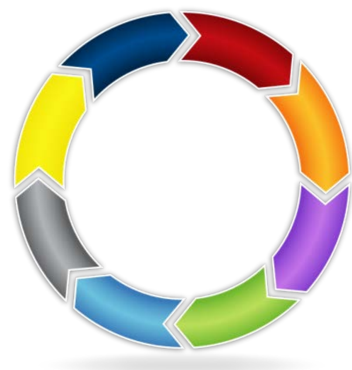
The degree to which computational models may be independently checked is clearly a function of adherence to principles of good coding practice, including transparency and modularity.

Finally, as so often in computational research, *the code is the model*, there are obvious ethical considerations relating to the balance between intellectual and commercial ownership on the one hand and scientific progress on the other hand. Codes, after all, can be copied easily. A code developed by one team of computational researchers for turbulent fluid dynamics might be incorporated by a second team in a larger, more complex code to simulate airflow over a turbine blade of a jet engine. It is clearly desirable to understand the extent to which accepted practice in computational modeling and coding allows for recognition of precedence for individuals' efforts, as well as possible commercial development, while safeguarding the public interest.

Recommendations

Responsible conduct of computational modeling and research rests on principles of transparency and accessibility coupled with carefully constructed plans for documentation, model evaluation, and model management. Standards of practice may identify mechanisms whereby modelers can express candidly the limitations of their computational models, methods, and results, without detracting from the opportunity to be informed by model predictions.

In the report *Models in Environmental Regulatory Decision Making* (Committee on Models in the Regulatory Decision Process, National Research Council, 2007), it is recommended that a coherent approach to model integrity and transparency rely on the development of a *life-cycle model evaluation plan* that "at a minimum…



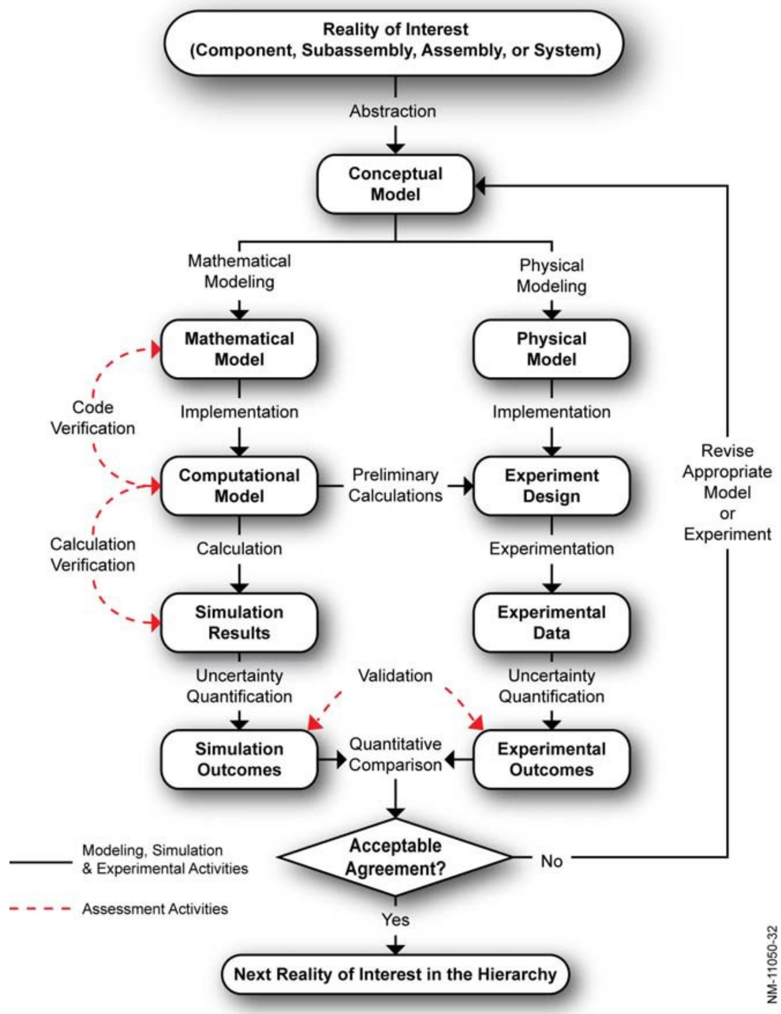
- Describe[s] the model and its intended uses.
- Describe[s] the relationship of the model to data, including the data for both inputs and corroboration.
- Describe[s] how such data and other sources of information will be used to assess the ability of the model to meet its intended task.
- Describe[s] all the elements of the evaluation plan by using an outline or diagram showing how the elements relate to the model's life cycle.
- Describe[s] the factors or events that might trigger the need for major model revisions or the circumstances that might prompt users to seek an alternative model. These could be fairly broad and qualitative.
- Identif[ies] responsibilities, accountabilities, and resources needed to ensure implementation of the evaluation plan."

Here, the exercise of formulating and documenting the responses to each of the bulleted items forces the model developers to i) identify primary and secondary stakeholders, ii) the degree to which the stakeholders' interests are represented by the model development, and iii) the consequences to the stakeholders of decisions and actions that may result from the model predictions. In its recommendations, the Committee “recognizes that the resource implications for implementing life-cycle model evaluation are potentially substantial. However, given the importance of modeling activities in the regulatory process, such investments are critical to enable environmental regulatory modeling to meet challenges now and in the future.”

The description of the intended use of a computational model should not be limited to the reality of interest with which it is concerned, but should include also the contributions that the model predictions have on decisions and judgments made in a regulatory or commercial context. The inevitable uncertainty associated with model assumptions, inputs, and coupling across system hierarchies suggests a “weight of evidence” approach (Committee on Models in the Regulatory Decision Process, National Research Council, 2007), in which the predictions of a computational model contribute to, but do not exclusively determine, a suitable action. In this context, a life-cycle model evaluation plan should include a description of the statistical analyses that will be undertaken to evaluate the contributions of uncertainty on model predictions, as well as an *a priori* mutually agreed upon mechanism for communicating this uncertainty.

> *“Effective uncertainty communication requires a high level of interaction with the relevant decision makers to ensure that they have the necessary information about the nature and sources of uncertainty and their consequences.”* (Committee on Models in the Regulatory Decision Process, National Research Council, 2007)

Computational models of a mechanistic nature, in which fundamental physical principles are reduced to well-understood conceptual models and, in turn, to extensively-documented mathematical models, may be amenable to a detailed paradigm for model verification and validation (V&V), as developed in a series of standards, published by the American Society of Mechanical Engineers, including the Guide for Verification and Validation in Computational Solid Mechanics (Performance Test Code Committee 60, ASME, 2006) from which we reproduce Fig. 4 below with permission.



Here, one distinguishes between verifying that a computational model faithfully encodes the desired mathematical algorithm and validating the model behavior against a reality of interest. A *verification and validation plan* formulated in advance of the design and performance of any validation experiments should include a description of "the approach that will be taken to verify the model" and "at a minimum…

- A detailed specification of the intended use of the model to guide the V&V effort;
- A detailed description of the full physical system, including the behavior of the system's parts both in isolation and in combination; and
- A list of the experiments that need to be performed [including a selection of data to be collected, metrics to be applied, and accuracy requirements to be imposed]."

As described in (Performance Test Code Committee 60, ASME, 2006), and highlighted in the illustration above, the design of validation experiments should be informed by the computational model development and vice versa, suggesting reasonably close collaboration between the teams involved with either task. Care should be taken however, that "experimental results…not be given to the modeler to preclude inadvertent or intentional tuning of the model to match experimental results."

Often overlooked, the tasks of code and calculation verification serve to ensure that the ability of a model to reflect the reality of interest is not impeded by non-fatal errors in the encoding that allow computation to proceed, but in ways that deviate measurably from the behavior predicted by a strict mathematical analysis. In cases, where the computational model implements a discretized solution algorithm for an infinite-dimensional problem, say an ordinary or partial differential equation with suitable boundary conditions, rigorous estimates on convergence rates with respect to discretization parameters may be used to challenge the accuracy of the model encoding.

With large development teams and multiple generations of model development, good software quality assurance (SQA) practice calls for a mutually agreed upon *change control management plan* among the developers and intended users of a computational model for tracking and documenting significant revisions to the model encoding, and for providing a digital repository of past versions of the model, together with relevant input data.

Models used for regulatory purposes or for procurement and development decisions made by government institutions, within the constraints imposed by their proprietary nature, should be available for peer review beyond basic documentation and simulation results, also after the intended purpose has been met. In the realm of scientific publishing, existing platforms are being retooled to support supplementary information in the form of computational algorithms and data. In both cases, change control management practices ensure a traceable record that can be revisited when new information or data becomes available, possibly warranting modifications to a model or to the quantification of uncertainty in its predictions. Such practices also instill confidence in research models (Waltemath, Henkel, Hälke, Scharm, & Wolkenhauser, 2013) and contribute to a comprehensive view of transparency and accessibility across all aspects of model development and use.

In instances of competitive bidding in response to requests for proposals (RFPs), a buyer of a computational model or designs and products obtained using a computational model could include expectations of traceability and change control management in the RFP, in an effort to reduce the moral hazard associated with less technical know-how.

“Models are developed and applied over many years by participants who enter and exit the process over time. The model origin and history can be lost when individual experiences with a model are not documented and archived. Without an adequate record, a model might be incorrectly applied, or developers might be unable to adapt the model for a new application. Poor historical documentation could also frustrate stakeholders who are interested in understanding a model… Each documentation should have the model’s origin with such key elements as the identity of the model developer and institution, the decisions on critical model design and development, and the records of software version releases. The model documentation also should have elements in ‘plain English’ to communicate with nontechnical evaluators. An understandable description of the model itself, justifications, limitations, and key peer reviews are especially important for building trust.” (Committee on Models in the Regulatory Decision Process, National Research Council, 2007)

CASE STUDIES

MATRIX PHARMACEUTICALS

Part 1:

Dr. Smith is a leading researcher in the design and fabrication of polymer-based pharmaceutical nanoparticles, as well as the development of novel protein-based pharmaceuticals. His lab is an exciting collaborative environment where some graduate research assistants work on developing computational models of protein structure interactions; other students work on using this modeling software to come up with new proteins that might make promising new pharmaceuticals; and still more graduate students work on creating and testing these proteins. In this collaborative environment, students help each other, and students often rely on the work of others. There is an expectation in the lab that students' work may be shared and applied to other projects. Dr. Smith is a popular thesis advisor with many students. Most students in his lab are able to get jobs in the pharmaceutical industry, and most of the research in Dr. Smith's lab is funded by pharmaceutical companies looking to develop the next wonder drug.

Nanoparticles are intriguing in that they offer ways to package a pharmaceutical compound to control the release profile of the drug. Dr. Smith originated an idea for modeling the interaction of the nanoparticle polymer components and protein-based pharmaceuticals mathematically. With funding from Matrix Pharmaceuticals, Dr. Smith hired Mr. Anderson as a graduate research assistant to implement this mathematical formulation in a computational model of the nanoparticles. Mr. Anderson is a bright and talented programmer with an undergraduate degree in computer science, but his organizational skills are not as developed as his creativity as a programmer. For his M.Sc. thesis project with Dr. Smith, Mr. Anderson created a code that embeds Dr. Smith's mathematical formulation in a nonlinear optimization algorithm. This algorithm is particularly fast for systems with sparse characteristics, but can be problematic for non-smooth objective functions.

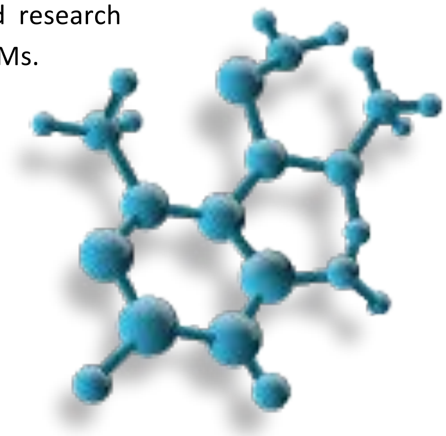
Mr. Anderson is a bright and talented programmer with an undergraduate degree in computer science, but his organizational skills are as developed as his creativity as a programmer.

As Mr. Anderson began writing his code, he was in a hurry, as he had already accepted an offer for a position with Zion Pharmaceuticals, to begin work two months later. He didn't bother to document the code while writing it, since he believed he would have time to do that later, while writing the thesis. The code is contained in a single file rather than broken down into modules, and is very hard for anyone other than Mr. Anderson to follow. Mr. Anderson was able to validate the code against the nanoparticle polymer-protein formulations already created in Dr. Smith's lab. The software correctly predicted their size and material properties. While he was finishing his work in the lab and preparing for his new job, Mr. Anderson assured Dr. Smith that he would be able to get the code commented and the M.Sc. thesis written within the first month of working at Zion. However, Mr. Anderson has found the job to be very demanding and, consequently, has not made as much progress as planned.

Matrix Pharmaceuticals has asked Dr. Smith to design a new nanoparticle-vaccine formulation for the treatment of HIV in the hope that such a formulation might hold the key to a potential vaccine. Dr. Smith thinks that Mr. Anderson's code would be very useful for this project and is considering asking another student to begin working on the project.

Part 2:

Ms. Trinity is a new student in Dr. Smith's lab. For her M.Sc. thesis project, she has been asked to take Mr. Anderson's software and design a new nanoparticle-vaccine formulation for the treatment of HIV. Because Matrix Pharmaceuticals requires a progress report due at the end of the month, Dr. Smith stresses to Ms. Trinity the importance of showing some good results to ensure continued funding. Such funding will enable Dr. Smith to give Ms. Trinity a paid research assistant position for the next year. Neither Ms. Trinity nor Dr. Smith is aware of how Mr. Anderson used the novel algorithm or its implications for their problem. Mr. Anderson knows they are using his code, but has started his new job and has been too busy to finish commenting the code. Since the code is not commented and is very large and complicated, it is difficult for Ms. Trinity to figure out what the code is doing. She decides to trust Mr. Anderson's software and begins designing the new formulation.



Using the software she tries a variety of polymer-protein compounds for the vaccine formulation. She finds that several of these compounds seem to correspond to very unusual predictions, but finally settles on one polymer that the software predicts will result in desirable nanoparticle characteristics. When she proceeds to create formulations with this polymer in the lab, the resulting nanoparticle properties are close to the predictions of the software. However, when she tries some of the formulations that had unusual predictions, she finds that actual nanoparticles have much better properties than those predicted by the software.

Ms. Trinity believes something is wrong with the software and doesn't know what she should do to correct it. She has been unable to contact Mr. Anderson to get help with his code. She thinks that maybe she should just report the one polymer for which the software predictions agree with her experimental findings to Dr. Smith for inclusion in the progress report. However, she worries that the disagreement between the computational predictions and the experimental observations made for several of the other polymer compounds may mean that all the predictions are problematic.

Questions for Part 1:

1. What should Dr. Smith do?

2. What are Mr. Anderson's obligations, if any, in this case?

3. What ethical issues can you identify at this point?

Questions for Part 2:

1. What should Ms. Trinity do?

2. Does Mr. Anderson bear any responsibility for Ms. Trinity's issues?

3. Is Ms. Trinity responsible for knowing how the software works?

4. What is Dr. Smith's responsibility to Ms. Trinity?

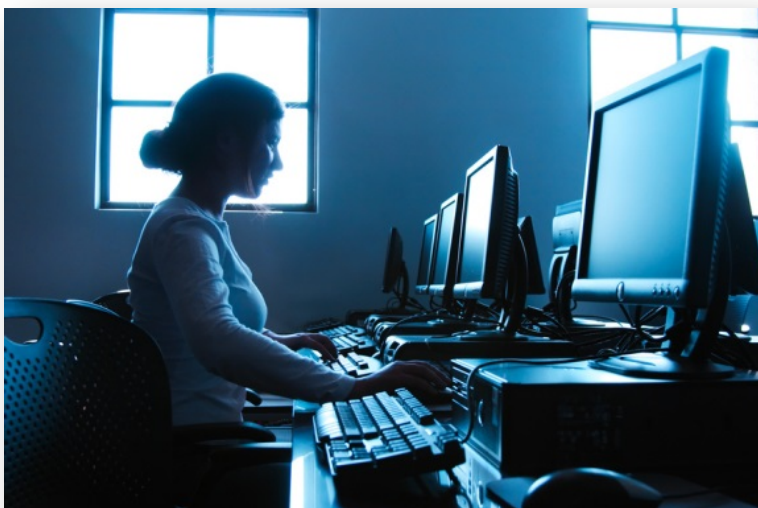
Real-life ethical situations rarely come with access to all the facts that would eliminate the need for judgment and leave a clear course of action as the obvious response.

Open-ended questions invite critical evaluation of the available information.

JASON'S DILEMMA

Part 1:

Regina Whipple is a recent graduate of a research group with a strong reputation in computational modeling of multistate solid mechanics simulations. This group relies on innovative approaches to bridging the gap between continuum and atomic length scales that couple density functional theory with tensorial smoothing approximations. While working for her dissertation, Regina invented an alloy analysis tool that she found capable of producing highly accurate predictions for the dependence of tensile strength on the distribution of dislocations and voids. Regina was able to document this work in a significant journal publication and was given several opportunities to have this work disseminated at international conferences.



Based on the reputation earned as a result of this work and its potential impact, Regina was able to realize her long term goal to secure a tenure-track position at a private and very prestigious institution. Although she never saw the letters of reference written on her behalf to supplement her job applications, she was told by members of the hiring committee that they were particularly impressed by the strong endorsement in these letters of Regina's scientific and computational skills and, in particular, their successful application to the alloy-design problem.

As part of her start-up package, Regina is given funding to support several graduate students through research assistantships. She is able to quickly recruit Jason, a particularly bright computer-science graduate and assigns to Jason the task of familiarizing himself with the theoretical work Regina did for the development of her code, as well as its implementation. Jason quickly assimilates this material and, with Regina's blessing and encouragement, creates an online repository for the code and several demonstration examples of its application. Regina begins to share information about this web-based repository with colleagues in academia and industry. Soon papers that rely on Regina's code applied to a variety of different alloy-design settings begin to appear in the literature.

In the process of preparing for his dissertation proposal exam, Jason comes across a segment of the code that appears perplexing. Here, a scaling transformation is applied based on a kharkovian limit, but Jason believes that this is done in a manner that may violate fundamental constraints on the decay rate of the elastic energy potential. When Regina is informed, she at first expresses serious doubts about her student's conclusions. Although she is eventually convinced that this apparent modeling error is a serious deficiency of her code, Regina thinks that since it appears to be of insignificant consequence to many, or possibly all, of the applications considered thus far, perhaps no amendments or notifications on the website are necessary. Jason is not so sure.

Jason believes that this is done in a manner that may violate fundamental constraints on the decay rate of the elastic energy potential.

Part 2:

At the same time, Dr. Smalley, at another university, is excited to learn about Regina's model through some conversations with colleagues. He believes he can use the model to examine the mechanics of foams that he has been creating in his lab for use in making lightweight wings for the aerospace industry. Dr. Smalley is particularly glad to see that Regina's code is available to other researchers via the repository.

Dr. Smalley is not an expert at computational modeling of solid mechanics, but Regina's software is fairly easy to use and he is able to develop some models of his foams that seem realistic and match some simple experimental compression and tension tests of a group of foams with different void properties. He doesn't know about the issue of the decay rate constraint error, or whether it could influence the predictions of fatigue failure of the foams. Fatigue is an important issue for aerospace materials, as it can lead to catastrophic failure of an aircraft in flight. Dr. Smalley plans to use the model's predictions to design new foams that he will then create in the laboratory for a large aircraft company.

Prior to proceeding with this plan he posts a note on Regina's website repository stating his intention to apply the code to an aerospace setting. When Jason reads the note he becomes concerned that errors from the violation of the decay rate constraint might indeed be relevant in this application. However, when he raises his concern with Regina, she replies that she is occupied with other projects and that, anyway, she is not responsible for policing the now numerous different applications of the code.

Questions for Part 1:

1. What should Regina do and why?

2. Since the error doesn't affect any of their results, is the existence of this error in the code a problem?

3. What do you think about the colleagues who might use the code from the repository for their own projects?

Questions for Part 2:

1. What should Jason do?

2. Does Regina have any responsibility to Dr. Smalley or for any of Dr. Smalley's results?

3. What should Dr. Smalley be doing?

"Engineers uphold and advance the integrity, honor and dignity of the engineering profession by…being honest and impartial, and serving with fidelity their clients (including their employers) and the public…"

(ASME Code of Ethics of Engineers, 2012)

TUNNEL VISION

Part 1:

Barnaby Baluster is a professor of civil engineering at Great Prairie University. Baluster and several generations of his graduate students have worked for more than a decade to develop accurate computational models for tunneling and excavation. All of the software for these computational models was written by graduate students. The initial development of the models was supported by a seed grant from Great Prairie University, then by research grants from the National Science Foundation. Since the initial development of the original open-source code, the code has been rewritten several times.

Baluster founded a consulting firm, Baluster and Associates (B&A), which uses the computational models to provide services to geotechnical engineers. Although former graduate students handle the day-to-day operations of B&A, Baluster remains actively involved as a principal of the firm. He spends about one day per week on B&A business. Baluster arranges for his graduate students to be employees of B&A. Contracts obtained by B&A become thesis projects for master's students. New kinds of tunneling methods become opportunities for research by doctoral students. This arrangement provides funding, professional experiences, and thesis and dissertation topics for Baluster's graduate students.

Ellen El-Hakim is one of Baluster's doctoral students. Throughout her graduate studies, she has been employed by B&A, and her dissertation project has resulted in a new computational model for simulating the torsional buckling of tunnel supports. After completing the doctorate, about two years from now, Ellen plans to pursue an academic career at a research university, continuing the work that she began at Great Prairie University and B&A. Ellen knows that to obtain an academic position, she must publish several articles from her doctoral work. Because the work is proprietary, however, B&A does not want Ellen to publish it.

Her dissertation project has resulted in a new computational model for simulating the torsional buckling of tunnel supports.

Part 2:

Desert City was once a small town on the interstate highway. As the population of Desert City has grown, so has traffic congestion. To improve the flow of traffic, the city has decided to relocate part of the highway underground. For the highway project, Desert City has selected Consummate Construction Consultants (CCC) as the lead engineering firm. The geotechnical engineers at CCC are deciding between two tunneling methods: cut-and-cover and the New Australian Tunneling Method (NATM). In cut-and-cover, first a trench is dug, and then support walls are installed. In NATM, a thin concrete lining is sprayed for support as soon as possible after the ground is opened.

The CCC engineers contract with Baluster and Associates to help them decide between

cut-and-cover and NATM. B&A assigns Amanda Ahn, one of Baluster's first-year graduate students, to work with the CCC engineers. The B&A cost analysis model indicates that for the Desert City site, the NATM would be significantly less expensive, and the stress analysis model indicates that the NATM should be able to handle the expected loads, but the CCC engineers feel uneasy about the results. Carefully examining the stress analysis model, Amanda discovers that for NATM, the model assumes that the concrete supports are installed instantaneously, without allowing the ground to settle first. Amanda believes this assumption might lead the model to calculate lower deformation of supports and lower stress values than would actually occur. As a first-year graduate student with little prior professional experience, however, Amanda is unsure about her findings.

Questions for Part 1:

1. What are the responsibilities of Great Prairie University and Baluster?

2. What should Ellen do to publish her research?

3. What rights does Ellen have to the code that she has written?

4. What are the rights of the developers of the original open-source code created with the support of the National Science Foundation?

Questions for Part 2:

1. What should Amanda do? For what reasons?

2. If Amanda decides to blow the whistle, how should she proceed?

3. What are the responsibilities of Desert City and the CCC engineers?

4. Does Baluster have any obligations in this case?

The Bayh-Dole Patent and Trademark Law Amendments Act of 1980 enables universities and small business recipients of federal funding to seek protection and ownership of inventions generated using this funding.

(Electronic Code of Federal Regulations; Patents, Trademarks, and Copyrights)

CIVIC CENTER

Part 1:

When plans are announced to design a new arena in Springfield, engineering firms bid competitively for the opportunity to complete the project. Company A manages to secure the job by assuring the city of Springfield that the company's use of computational models will allow them to complete designs for the arena in less time and at less cost than competing firms could. In determining their design time, Company A estimates that it will take four weeks to develop the computational model.

Bill is leading the team that is developing the computational model that Company A will use to test their designs. The team progresses quickly at first, and soon the code is able to successfully match the expected forces and deformations of a variety of standard benchmark cases. However, they find it difficult to incorporate a thorough buckling analysis into the model. The most accurate method for determining buckling loads requires the solution of a complicated nonlinear problem involving details such as beam imperfections and plastic deformation. However, attempts to include this complex analysis into the model result in simulations running too slowly to be practical. Bill's team spends a significant amount of effort working on this problem, but ultimately is unable to reduce the run time enough to include this method of buckling analysis.

Working under the pressure of Company A's promised deadline, Bill makes a decision to incorporate buckling through a simplified eigenvalue analysis. This analysis assumes that all deformation is perfectly elastic and uses simpler modeling of beam properties, allowing buckling loads to be determined by solving a relatively simple linear eigenvalue problem. This buckling approximation is non-conservative: it overestimates yield buckling loads. After extensive testing Bill has determined that this approximation is within an acceptable margin of error for the small deflections expected from designs. With this final issue resolved, Bill is able to present his completed model to Company A within the four-week deadline.

Part 2:

Jean leads the team charged with using Company A's computational model to evaluate potential arena designs. Bill's team has provided extensive documentation of the computational model, so Jean is aware of the model's limitations, including the approximation used for predicting buckling failure and the range of deflections for which the approximation is valid. Jean validates the model against standardized benchmark cases and is satisfied with the results, including the buckling analysis.

Jean worries that the deflections may be too large for Bill's buckling approximation.

Jean's team is given two different designs to test using the computational model. Both designs are space frame trusses, consisting of beams arranged in a repeating pattern of pyramid-like structures. The first design is a simple structure that uses less material and will be easier to construct. The second design is similar to the first, but also contains additional reinforcing members. The reinforcements are intended to make the second design stronger, but the extra material and more complicated construction make the reinforced design significantly more expensive to build.

When Jean's team tests the designs, the computational model predicts that both designs can handle all required loading configurations without failure. However, upon examining the results more closely, Jean finds that the beams in the simple design experience some deflections that she worries may be too large for Bill's buckling approximation. Jean is unsure how she should proceed. The model demonstrates that the reinforced design will not fail, but Jean does not want to recommend the more expensive design, if it is possible that the simple design might work.

Questions for Part 1:

1. What are the responsibilities of Company A during the bidding process?

2. How can Bill justify the use of the simplified buckling analysis?

3. What are the responsibilities of the City of Springfield?

Questions for Part 2:

1. What should Jean do?

2. What are Bill's responsibilities to Jean's team?

3. What expectation does the City of Springfield have?

"A profession is not a business. It is distinguished by the requirements of extensive formal training and learning, … a code of ethics imposing standards qualitatively and extensively beyond those that prevail or are tolerated in the marketplace,…and, notably, an obligation on its members …to conduct themselves as members of a learned, disciplined, and honorable occupation"

355 N.Y.S. 2d 336 (1974), cited in (Schwartz, 2004)

TOOLS FOR ASSESSMENT

FORMATIVE ASSESSMENT

A decision procedure checklist (Keefer, Wilson, Dankowicz, & Loui, 2013, to appear) helps in the writing of case responses that thoroughly address four key concepts relevant to the analysis of complex ethical cases, namely the identification of 1) ethical issues and responsibilities, 2) relevant information, 3) alternative courses of action, and 4) consequences of action. Such a checklist enables ongoing formative assessment of the written responses as they are composed, and it prompts examination of details that may have been initially ignored.

Decision Procedure Checklist (DPC)

- *Ethical issues/professional responsibilities identified*
  - *Have the primary and secondary stakeholders been identified? Stakeholders include individuals, groups, societies, companies, etc.*
  - *Have the ethical issues and how they relate to various stakeholders been identified and considered?*
- *Additional information identified*
  - *Has additional useful knowledge or information concerning the problem been identified?*
  - *Are any additional resources identified that could help in developing a solution to the problem?*
  - *Have actions been taken that could provide additional useful information or provide additional resources?*
- *Consideration of the actions taken*
  - *How well do recommended actions address the concerns of primary and secondary stakeholders?*
  - *How well do the recommended actions address the ethical issues identified?*
  - *Are there any creative "middle way" courses of action that can address more than one ethical issue?*
- *Consideration of long and short-term consequences*
  - *Is there consideration of how the proposed solution might affect the stakeholders in the problem over time?*
  - *Have any morally significant longer-term consequences of the proposed solution been considered (including possible accidents, misuses, etc.)?*

SUMMATIVE ASSESSMENT

A decision procedure scoring guide (Keefer, Wilson, Dankowicz, & Loui, 2013, to appear) provides a means of assessing the proficiency with which responses address the four key issues presented in the checklist. The scoring guide may be used in a purely qualitative manner, or it may be used quantitatively by assigning numerical scores to responses (e.g. 1 point for less proficient responses, 2 points for proficient, and so on). The numerical score enables the student to more easily track her progress through each part of the case or through multiple cases, and allows an instructor to readily evaluate overall performance.

Decision Procedure Scoring Guide

Ethical issues and professional responsibilities:

Expert	*More Proficient*	*Proficient*	*Less Proficient*
Identifies the relevant ethical issues in the case and how they relate to professional responsibilities. Identifies and tracks concerns of primary and secondary stakeholders.	Identifies more than one ethical issue and/or a professional responsibility. Identifies and tracks concerns of the primary stakeholders.	Identifies a key ethical issue and/or a professional responsibility. Identifies the concerns of a primary stakeholder.	Identifies only a single ethical issue or does not consider the problem to have an ethical dimension.

Additional information and resources:

Expert	*More Proficient*	*Proficient*	*Less Proficient*
Recognizes and makes appropriate use of resources that support ethical action (or that fail to). Identifies additional significant knowledge or information that might be useful to know for identifying appropriate action.	Recognizes some resources that might support ethical action. Identifies some additional knowledge or information that is useful and is incorporated into the proposed solution.	Considers some potentially useful information, but does not effectively incorporate the information into the solution. Additional resources are not considered.	Does not recognize or incorporate additional resources and information into the proposed solution.

Alternative courses of action in response to the case:

Expert	*More Proficient*	*Proficient*	*Less Proficient*
Recommends course of action that addresses several ethical issues simultaneously, and proposes solution that addresses and tracks the concerns of relevant stakeholders.	Recommends course of action that addresses more than a single ethical issue effectively, and proposes solution that addresses the concerns of more than a single stakeholder.	Recommends course of action that addresses a single ethical issue effectively, and proposes solution that addresses the concerns of a single stakeholder.	Recommends course of action that does not address a key ethical issue effectively, and proposes solution that does not adequately address the concerns of any stakeholders.

Long and short-term consequences of proposed solutions:

Expert	*More Proficient*	*Proficient*	*Less Proficient*
Proposed solution anticipates morally significant short and longer-term consequences of actions. Morally significant alternative actions are conside-red anticipating changing circum-stances or events.	Proposed solution recognizes some morally significant short and longer-term consequences of actions. Some alternative actions are considered anticipating changing circumstances or events.	Proposed solution recognizes some morally significant consequences of actions.	Proposed solution does not recognize morally significant consequences of actions.

RESPONSES AND COMMENTARY

MATRIX PHARMACEUTICALS

SAMPLE RESPONSE[1]

Part 1:

Ethical issues/professional responsibilities

The primary stakeholders are Dr. Smith, Mr. Anderson, and Matrix Pharmaceuticals. Mr. Anderson was obliged to provide annotations for the code he wrote during his employment as a GRA, and when responsibilities leading up to graduation mounted up he then agreed that he would write the notes after he began his new job. Because he is no longer an employee of Dr. Smith, he does not have any formal obligation to provide the notes, but it would be professional and courteous to make good on his earlier agreement. Dr. Smith, for his part, does have an obligation to honor intellectual property rights to the code written by Mr. Anderson, and to maintain appropriate attribution of the work in publications and in future research. Matrix certainly has an interest in furthering research with the software because it could benefit their HIV project.

Another issue is that Mr. Anderson is now employed by another company (Zion Pharmaceuticals) which could be researching projects similar to Matrix Pharmaceuticals, and could constitute a conflict of interest for Mr. Anderson.

A secondary stakeholder is the portion of society that is susceptible for contracting HIV, because the development of an effective vaccine may be greatly benefitted [sic] by the development of Mr. Anderson's software.

Additional information for full assessment

It would be helpful to know what the formal terms of Mr. Anderson's employment were under Dr. Smith, in case there may be a legal obligation for Mr. Anderson to complete the notes. Also, was any sort of copyright, patent, or other formal intellectual property right proceedings enacted for the code that was written? In addition, does Matrix Pharmaceuticals or another funding source for Dr. Smith's research have any rights to

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[1] This is an actual student response from a participant in an RCR study at the University of Kansas, conducted with approval from the university's Institutional Review Board.

obtain the code annotations as part of a contract or grant agreement? Finally, is there a formal obligation for Mr. Anderson to not contribute to work that could directly benefit a competitor (Matrix) to his current employer, Zion Pharmaceuticals?

Alternative courses of action

It is possible (1) for Dr. Smith to just cut his losses with Mr. Anderson, and to task another GRA with developing the code further, without further consultation with Mr. Anderson. This would remedy the interests of Dr. Smith and Matrix Pharmaceuticals., but does nothing to address Mr. Anderson's interest in his prior work. (2) Dr. Smith could press Mr. Anderson to honor his verbal agreements and provide the notes. This could facilitate the new research, and would force the interaction with Mr. Anderson, potentially causing problems with his current employer. (3) Dr. Smith could consult with Mr. Anderson and ask him to brief the new GRA with respect to important features of the software, begin development of the code, and retain recognition of Mr. Anderson's work and any associate intellectual property rights. This would allow Mr. Anderson to hand off any responsibility, facilitate new research, and also save him from excessive distraction from his current job. It is not likely that this would cause a conflict of interest with his current employment, and would address the concerns for Dr. Smith and Matrix.

Long and short term consequences

If Dr. Smith proceeds with research without consulting Mr. Anderson (alternative-1), it is possible that an intellectual property dispute could arise in the future, and could slow any progress made with Mr. Anderson's code. If Dr. Smith attempts to press Mr. Anderson (alternative-2) it is quite possible that Mr. Anderson will just ignore the requests, or if he does honor his earlier agreement, he could have some problems with his current employer for contributing to research funded by a competitor. (alternative-3) If Mr. Anderson briefs the new GRA and cleans his hands of future responsibility he can retain recognition of his work, and be free of any conflicts of interest with his new employer. It is likely that the Smith group's development of the software will proceed quicker if this alternative is chosen, and the potential benefit to people at risk of contracting HIV will be advanced more readily.

Questions for Part 1:

1. Dr. Smith should consult with Mr. Anderson in order to brief the new GRA (alternative-3), maintain attribution of Mr. Anderson's work, and further the new research in the most expedient way.

2. Mr. Anderson’s may not have any official obligations, except that he ought to be professional and courteous in honoring his prior verbal agreement with Dr. Smith.

3. The issues at hand are intellectual property rights/attribution due to Mr. Anderson’s work (i), the interest of Dr. Smith and Matrix to proceed with the new research (ii), society’s potential benefit if the research is successful in developing a vaccine for HIV (iii), Zion’s potential interest in not having one of its employee’s assisting in research efforts of a competitor (iv).

Part 2:

Ethical issues/professional responsibilities

The primary stakeholders are Ms. Trinity, Dr. Smith, Matrix Pharmaceuticals, and Mr. Anderson. The individuals who could benefit from a HIV vaccine are secondary stakeholders. The issues at hand include the concerns found in Case 1, Part 1, but also include added responsibilities due to the progress report requirement of Matrix. Ms. Trinity has an obligation to provide a more or less full disclosure of recent results obtained with the software. Dr. Smith has an obligation to convey the essential elements of the results to Matrix, even if they are not as promising as desired.

Additional information for full assessment

To aid in the understanding of the software, an outside consultant could be hired to analyze the code. Also, it may be helpful to compare the predictions for Mr. Anderson’s software with those obtained by other similar programs.

Alternative courses of action

Ms. Trinity could (1) report only the single favorable result to Dr. Smith. This would mislead both Dr. Smith and Matrix. Ms. Trinity could also (2) report all the results to Dr. Smith with her critical assessment of the software. This could jeopardize her future as a GRA, but could be of ultimate assistance in preventing the waste of time and expense on research which may be futile. Another option (3) is that the outside software consultant and/or comparison with another software may identify problems with the software and allow it to be used for better predictions in the future.

Long and short term consequences

Alternative-1 may assure that Ms. Trinity has funding secured as a GRA for the next year, but if further positive results are not forthcoming, then Dr. Smith may nonetheless fire her, or Matrix may cut funding if the next progress report gives no hopeful results. Alternative-2 could result in ending the use of Mr. Anderson's software for HIV vaccine research and/or the loss of Ms. Trinity's job. However, it is also possible that Matrix would be understanding enough to give provisional support of further investigation into Mr. Anderson's code. Alternative-3 has the potential to get to the bottom of some of the mysteries surrounding the software, and further vaccine research for HIV, but it could also just be an additional waste of time and resources if the code remains just too complicated.

Questions for Part 2:

1. Ms. Trinity should make a few comparisons with other predictive software, and then should proceed with her full results and critical assessment. A negative finding, as this may be, is still a good finding if it averts the wasting of future resources.

2. Mr. Anderson should, to the best of his ability, provide a summary of important features of his software to Ms. Trinity so that her work can proceed.

3. Ms. Trinity cannot be expected to be responsible for understanding a complex software in a short time, especially if she is not a software engineer.

4. Dr. Smith should not put undue pressure on Ms. Trinity to produce good results, even with the threat of halting continued employment. Dr. Smith's responsibility to Mr. Anderson is to provide attribution for his work on the software, and to uphold any intellectual property rights that Mr. Anderson may have for the work.

MATRIX PHARMACEUTICALS COMMENTARY

The goal of any classroom discussion of a (possibly fictional) case related to responsible conduct is to allow students to practice moral reasoning skills around key topics (in these cases topics in computational modeling). A successful discussion is one in which the students are able to:

1. Identify the relevant issues that exist in the case;
2. Identify the various parties (or stakeholders) that play a role or are impacted by the case;
3. Explore a number of potential actions and their consequences; and
4. Arrive at a reasoned course of action.

There are a number of approaches that can be taken to achieve such a discussion. The best approach may depend on the skill level of the participants, with more novice participants benefiting from a more structured approach, while experienced participants may be able to carry a discussion with just a few leading questions.

For a structured approach, it often helps to start with four columns on the board labeled: Issues/Professional Responsibilities, Stakeholders, Actions, and Consequences.

Issues/Professional Responsibilities:

For the Matrix Pharmaceuticals case, key issues that should be identified by the participants include:

- Model integrity (limitations of the numerical method): Limitations of the optimization algorithm for non-smooth objective functions and the potential of these limitations to cause erroneous results appear, by the description in this case, to be the source of Ms. Trinity's problems. These limitations are not understood by Ms. Trinity at this point and have not been communicated to her as a user by the developer, Mr. Anderson.

- Model integrity (validation and verification): In addition to the fact that the limitations of the algorithm have not been documented, the described validation appears insufficient. Mr. Anderson has validated the model against a limited set of experimental data, but Ms. Trinity is applying the model beyond that range of validation. There is also little discussion of the verification of the encoding. It is possible there are other computational or coding errors.

- User responsibility: When a user relies on a computational model developed by someone else (whether obtained from a commercial source, an open source, or a colleague), the user takes on a responsibility to use that model appropriately. Not doing so risks erroneous results that can have downstream consequences (in this case, the potential for poorly designed drug formulations that might have health consequences to patients). Dr. Smith and Ms. Trinity have an obligation to understand key aspects of the code they are using. Without such understanding, their nanoparticle design work may be hindered.

- Developer responsibilities: Mr. Anderson has an obligation to create code that is clearly documented and where limitations of the code are identified. Without this documentation, it is difficult for users (including Mr. Anderson) to operate the model appropriately. One twist in this case is timing. Mr. Anderson has not completed his work, but may plan to finish his thesis work eventually. Ms. Trinity, on the other hand, needs this documentation now.

- Student and employee responsibilities: Mr. Anderson had obligations related to his employment as a graduate research assistant. There is an expectation that he will complete his thesis and research work. However, it is not uncommon for students who move into employment before completing a thesis to never finish.

- Employee responsibilities: Mr. Anderson now has obligations to his current employer.

- Academic advisor responsibilities: Dr. Smith has a responsibility to guide Ms. Trinity and Mr. Anderson as an academic research advisor and employer. This is part of his employment as a university professor.

- Contract/Funding responsibilities: Dr. Smith has obligations to the industrial sponsor, including his obligations to make progress and to communicate the research results clearly and honestly. Not living up to these obligations could result in the termination of funding.

Other issues that could be discussed include:

- Conflict of interest: Mr. Anderson's responsibilities to his new company, his previous sponsor, and his research advisor could result in a variety of conflicts including the sharing of proprietary information with the new company.

- Ownership of the code and intellectual property: The code itself can be considered as intellectual property whose ownership is shared by Dr. Smith and Mr. Anderson. As employees of the university, the university will likely have some ownership interest as part of the employment contract. Matrix Pharmaceuticals may also have some ownership interest as stipulated by the sponsorship contract. If Mr. Anderson planned on using the code at Zion, there could be issues related to this ownership.

As with many cases, this case includes issues specific to computational modeling (such as model integrity and user/developer responsibilities), as well as issues that are more general (such as issues of academic advising, industrial research sponsorship, and employment).

Stakeholders

It is important to make sure that all stakeholders (in particular those not already named in the story) are identified. For this case, key stakeholders include:

- Ms. Trinity, Mr. Anderson, Dr. Smith
- The industrial sponsor of the research, Matrix Pharmaceuticals
- Mr. Anderson's new employer, Zion Pharmaceuticals
- The university
- Patients that might benefit from a new pharmaceutical
- Future students in Dr. Smith's lab

Actions and Consequences

The questions at the end of each part of the case are directed towards the potential actions that might be taken by the stakeholders. With more advanced participants, one might start with these questions. Actions and consequences are closely connected. In this case, one is presented with a complicated situation that would not exist if prior actions had been optimal. As such, it is worthwhile to start the discussion of actions by discussing what should have happened (*prior actions*). Before filling in the actions and consequences, one might ask the question of "what should have happened?" or "how could these problems have been avoided?" Ideally, one should be able to get answers such as:

- Mr. Anderson would have commented the code and made it more readable by splitting it into simple modules. This would have made it possible for Ms. Trinity and Dr. Smith to identify what problems might occur with the new formulations.
- Mr. Anderson could also have communicated the limitations of the optimization algorithm to Dr. Smith and Trinity through the commenting in the code, through accompanying documentation (such as a user's manual), or through warning messages in the user interface of the software. This would, again, have made it easier for Ms. Trinity to identify the potential problems with the new formulations.
- Dr. Smith could have avoided this situation by being a more involved advisor to Mr. Anderson and insisting more clearly on in-line comments and stand-alone documentation while Anderson was still under his employ. He appears to have delegated too much of the responsibility for code development to Mr. Anderson and, as such, is not fully aware of what has been done. He also could have assisted more in the transfer of information from Mr. Anderson to Ms. Trinity.

Students discussing a case such as this will frequently have an easier time focusing on the obligations of faculty and employers than on the responsibilities of students like themselves. It is worthwhile to have them think about how they might act if they were the advisor and what factors might influence the advisor's actions. One can also have students bring into the discussion their own experience writing code in the laboratory, asking question such as "Do you discuss the algorithms you have used with your research advisor?" or "When you write code, would another student in the lab be able to interpret it easily?"

In exploring possible *future actions*, the case focuses primarily on what actions are available to Dr. Smith and Ms. Trinity. For Ms. Trinity, the case presents two potential actions:

- Reporting only the modeling results of the "good" formulation.

- Reporting all of the results and demonstrating the potential issues with the computational model.

The former action should be identified as lacking in transparency and honesty. The latter should elicit some discussion of potential consequences that could include loss of funding from the industrial sponsor. While the case puts these two actions forward, participants should be encouraged to think creatively and consider other possible actions. The case does not present the expectations of the industrial sponsor or what Dr. Smith might think about the findings. Participants should identify such additional information as missing from the case. Other potential actions include:

- Discussing the results with Dr. Smith and getting his input on how the results should be presented.

- Examining whether the progress report might be delayed to allow time for Ms. Trinity to investigate the model and better understand any modeling limitations.

One might expect some discussion of what might be asked and expected of Mr. Anderson. As he is no longer employed by the university and Dr. Smith, Mr. Anderson no longer has employment obligations (or the threat of losing employment if he fails to follow through). Dr. Smith can still require work to be completed for the thesis to be considered complete, but that may not motivate quick work on Mr. Anderson's part. It is not uncommon for students in Mr. Anderson's position to become so involved in their new job that they never complete a thesis. As such, it is risky for Ms. Trinity to rely on Mr. Anderson for her own progress.

Throughout any discussion, a goal of this case is to have the participants understand that algorithms have limitations that may make them inappropriate for use in solving some problems. A developer may have a responsibility to disclose such limitations to others that would use the model in order to prevent misuse. A user, similarly, has a responsibility to understand the potential limitations of computational model and its software encoding, so they do not misuse the software and end up with erroneous results. The complexity of the code and the embedded mathematical algorithms, the quality of documentation, and the quality of user interfaces can all factor into this transparency and disclosure between developer and user.

TUNNEL VISION

SAMPLE RESPONSE AND EVALUATION[2]

Part 1:

In this part, there are no ethical problems. Everyone benefits. Geotechnical engineers obtain consulting services from B&A. Students gain practical experiences. The university receives royalties from licensing the technology.

The university is responsible for educating students and for commercializing research for economic benefit. Baluster is responsible for supervising his graduate students the university and employees at the company.

Academic freedom means Ellen has right to publish her work. Since Ellen wrote the code, she can take it to another university. An exact copy of the final version of the code can remain at Great Prairie University. Developers of the original version of the code have the right to run that version of the code.

Part 2:

If the city chooses the NATM because it is cheaper, Amanda should blow the whistle because the safety of the public is the most important. She could post a video on YouTube to explain how the program is giving dangerous recommendations.

Desert City is responsible for providing fast and smooth commutes for its residents. CCC is responsible for fulfilling its contract with the city, such as choosing a good tunneling method.

As Amanda's adviser, Baluster is obligated to supervise her thesis research. As a principal of B&A, Baluster is obligated to maximize shareholder value.

Evaluation:

For both Part 1 and Part 2, the response is superficial. The lists of responsibilities and obligations of the main actors omit responsibilities to other affected parties such as

[2] This is a fictitious student response intended to demonstrate only a superficial level of understanding of the ethical issues.

ensuring the safety of construction workers. The response neglects the responsibilities of senior engineers to supervise the graduate students, and to ensure that the technical work is performed competently.

The response for Part 1 fails to identify Baluster's conflict of interest. As a principal of a firm that employs his students, Baluster has a role conflict in which his financial interests may influence or interfere with his responsibility to advise his students and to promote their professional development.

The response neglects intellectual property issues. The university probably holds a patent since the computational models were originally developed at the university. The university has then licensed that patent to B&A for commercialization. Since Ellen has been employed by B&A, she has likely signed an agreement that states that some or all of her work belongs to B&A. As a consequence, she may be restricted in what she can publish and what she can take to another university. When computational models are developed with industrial funding, all parties should first negotiate what might be published. Typically a published paper can describe the key ideas in the development of the model, but not the specific implementation. The paper can demonstrate the model with illustrative or fictitious data, not the proprietary data used by an actual client. At a minimum, Ellen should find out what her legal obligations are.

For Part 2, whistle-blowing should always be a last resort because it has serious detrimental consequences for everyone. As a first-year graduate student, Amanda probably has limited credibility and experience. She should first check with more senior, knowledgeable engineers, perhaps Baluster himself, to confirm her understanding.

Applying the Decision Procedure Scoring Guide, we can see that the response to Part 1 states there are no ethical issues, and the response to Part 2 identifies only one general ethical issue. The response does not identify any missing information or resources that would help make a good decision. The actions recommended by the response are inappropriate and do not consider long-term consequences.

CIVIC CENTER COMMENTARY

This fictional case study is inspired by circumstances surrounding the construction and collapse of the Hartford Civic Center. The Hartford Civic Center was constructed during 1972 and 1973, a time when computational modeling was still a new technique in engineering. The roof collapsed under heavy snow in the early morning on January 18, 1978. Investigation after the collapse revealed that the design was susceptible to buckling failure, and that buckling had not been considered in the computational model (Shepherd & Frost, 1995). In the fictional case study, the computational model does account for buckling to a degree, albeit by making assumptions that limit its applicability. Both the real-life example of the Hartford Civic Center and the fictional Springfield arena design demonstrate that a computational model “is a tool, and not a substitute, for sound engineering experience and judgment” (Shepherd & Frost, 1995).

Part 1:

The first part of the fictional case study covers the firm's bidding for the project and Bill's work on developing a computational model. Possible ethical issues include:

- The nature of the competitive bid made by Company A and the claimed advantage in terms of time to completion (and, consequently, cost) due to reliance on computational tools. It is useful to inquire as to the possible conflict that exists between Company A making an objectively informed bid that they believe can be met and the competitive character of the bidding process (Schwartz, 2004). Company A has responsibilities to its owners and shareholders that include maximizing profit while minimizing risk, e.g., that associated with legal action due to failure to consider consequences to public safety.

- The nature of simplifying assumptions made in the design of a computational model and efforts for verification and validation. Judgment and experience cannot be eliminated from the process of model development. Bill’s decision to include an approximate buckling formulation in the computational model allows Company A to meet its stipulated time commitment, but possibly at the expense of model validity. The case describes validation efforts against benchmark data, as well as testing used to establish the order of approximation and magnitude of likely errors incurred from the simpler eigenvalue analysis.

- The nature of efforts by Bill and Company A to disclose modeling assumptions and make documentation and encoding available for peer review and independent evaluation. As the awarding of the contract to Company A ultimately is a matter of public policy by representatives of the people of the city of Springfield, it is important to inquire as to the ability of these representatives and decision makers to make an informed decision on the construction of the Springfield arena. Independent peer review that might provide a traceable record of accountability might also be in conflict with the proprietary interests of Company A.

- The nature of conflicts between Bill's responsibilities as an employee of Company A and his responsibilities to his professional community. The pressure Bill feels to meet the stipulated timeline forces him to make decisions that serve the short-term bottom line, but increase long-term risks associated with uncertainties and lack of validation. The trustworthiness of computational models when used for public contracts might be put into question by decisions made in this single instance.

Although Bill is singled out as the principal actor in this part, key additional stakeholders thus include the people, elected, and appointed representatives of the city of Springfield; the owners and managers of Company A; Bill's coworkers on the development and design teams; competing engineering firms; the professional community of computational designers.

In exploring possible alternative past and future actions relevant to the first part of the case study, one notes the absence of information as to the organization of Company A's bidding process, the city of Springfield's process for selecting bids and awarding contracts, and Company A's project management implementation, including the degree to which Bill's superiors are made aware of the challenges faced by the development team and the decisions taken under the pressure of existing deadlines.

Possible past actions include adherence to sound principles of computational model development that include the development of a life-cycle model evaluation plan, encompassing plans for verification and validation, as well as change management control. Such an approach might improve the degree of communication within Company A during the development of a competitive bid, including the expectation that the allocated time would be the result of traceable internal deliberations. The city of Springfield could require that such a life-cycle model evaluation plan be made part of the bidding process. The plan could stipulate decision points for re-evaluation of project timelines and resource allocations, as well as internal checks and balances between Company A's development and management teams.

The eigenvalue analysis Bill used is a simple method to compute buckling loads in a finite element model. This method works by applying sample loads to the beam, then solving the eigenvalue problem $\lambda^f K_g \cdot \varphi = K_e \cdot \varphi$, where φ denotes a vector containing the nodal displacements, K_e is the global elastic stiffness matrix, K_g is the geometric stiffness matrix (which incorporates the beam's deformed shape), and λ^f is the load factor (Mahfouz, 1999). The smallest value of λ^f is the critical load factor, λ_{cr}^f which is the minimal factor that all loads must be scaled by to produce buckling failure. This analysis assumes an idealized, perfectly elastic beam, resulting in a linear eigenvalue problem which is relatively simple to solve. A typical nonlinear buckling analysis is an iterative process that works by gradually increasing an applied load until the system becomes unstable. This nonlinear analysis is more time-consuming than the eigenvalue approach, but it is also more accurate. Because of its less accurate and nonconservative nature, eigenvalue analysis is not recommended for real-world buckling problems.

For projects such as these, however, time is money, with additional bonuses being earned for completing work early or penalties being assessed for work that is completed late. Bill's decision to pursue a simplified buckling analysis may be warranted by pressures to meet stipulated deadlines, but if Bill feels that the time constraint is preventing him from creating a model of adequate quality, he should make this known to his superiors. Cost overruns and delays associated with a more comprehensive model might result in reduced short-term profit, but demonstrate adherence to sound modeling principles and concern for reputation and public safety.

Part 2:

The second part of the fictional case study covers the use of Bill's computational model for construction design decisions. Additional ethical issues include:

- The dependence on computational models for making "go" versus "no-go" decisions. Should a verified and validated model be used only to reject design decisions that are predicted to result in an undesirable outcome, or also to approve design decision that are predicted to result in a desirable outcome?

- The reliance on model predictions outside of documented ranges of validity. The integrity and trustworthiness of design decisions based on a computational model assumes that the model has been appropriately validated for the application. The influence of modeling assumptions and uncertainty, if not quantified for the specific operating condition, may pose unreasonable risks.

- The need to minimize cost while maximizing benefit for different stakeholders and across multiple timescales. Jean feels conflicted by the need to recommend a low-cost design solution even without a clear quantification of uncertainty and risk. Although this may result in short-term benefits for the company and the procurer, long-term costs could be substantial for all parties.

The case describes the due diligence employed by Bill and the development team in documenting the computation model and providing evidence for its trustworthiness within a specified range of operating conditions. It is clear that Jean's team is knowledgeable about all relevant aspects of the model and that they have conducted their own independent evaluation to build additional confidence in model predictions.

The opportunity to reevaluate a computational model with changing circumstances could be formalized in a life-cycle model evaluation plan. This would spell out the criteria that would necessitate model modifications and describe steps for further model validation. Jean's observations might warrant the inclusion of a more costly nonlinear buckling analysis, at least in a number of relevant sample test cases, in order to quantify model uncertainty in the two potential designs.

In the absence of further modeling work, Company A could rely on a "weight of evidence" approach, in which the computational model would only provide one piece of evidence in favor of, or against, a proposed design. Jean could disclose the issues that had been identified by the analysis to her superiors and make recommendations for additional physical experiments to build confidence in either of the proposed designs.

ROLE PLAYS

INTRODUCTION

Role-play is a powerful method for teaching topics in the responsible conduct of research (RCR). In the RCR role-plays developed by (Brummel, Gunsalus, Anderson, & Loui, 2010) and assessed by (Seiler, et al., 2011), each scenario has two speaking roles, a graduate student and a professor. The instructions for each role provide different perspectives on a common RCR problem.

Almost any realistic RCR scenario can be converted into a role-play. On the following pages, we provide a two-person RCR role-play based on Part 1 of the "Tunnel Vision" scenario. This role-play is a composite of incidents that actually occurred at our university.

An instructor can organize a two-person RCR role-play with any number of participants. First, the instructor tells the participants that the role-play experience will be valuable if they engage in the activity and play their roles authentically; the instructor assures the participants that there are no correct or incorrect ways to play the roles. The instructor organizes the participants into pairs. In each pair, one participant plays the role of the graduate student, and the other plays the role of the professor. Each receives instructions for only that role and takes time to prepare. If time permits, participants with the same role can meet in small groups to share ideas before starting the role-play.

The role-play itself can run for about ten minutes, typically enough time for the participants to identify the main RCR issues and to start thinking about ways to address those issues. The instructor then leads a discussion of the entire group. In addition to addressing the RCR issues, the instructor emphasizes the importance of communicating openly, understanding others' perspectives, and gathering information before acting.

TUNNEL VISION

ROLE PLAY

Graduate Student:

Because you have changed research advisers several times, you have taken a long time to start research for your doctoral dissertation. You have finally found a doctoral research adviser with whom you are happy. You are now finishing your fifth year of graduate studies, but you are making good progress in dissertation research, and your adviser thinks you could finish in one more year.

Originally you had planned to work in an industrial or government research laboratory after you completed the doctorate. As a consequence, you had not focused on publishing the results of your research so far. Now you are thinking of pursuing an academic career. To improve your competitiveness for an academic position, you need to improve your publication record. Consequently, you plan to remain a doctoral student for two more years.

For your dissertation project, you are developing and implementing computational models that simulate the behavior of tunnel supports under various loads. You plan to take the code that you developed with you when you begin your academic career so that you can continue research in the same area.

In the past, your research assistantship has been funded by a grant from the company that your adviser co-founded. For the next year, your adviser has told you that your funding will be split between a university research assistantship and a part-time internship at this company, which is located in town. Other doctoral students in your adviser's group are being offered the same opportunity. You are concerned that the internship duties will divert your attention from your dissertation work.

For your routine annual progress check, you are about to meet the new director of graduate studies in your department, with whom you have previously had little interaction. Prepare for your meeting.

Summary

- You are not on good terms with any faculty member in your department except your current adviser, with whom you are happy.

- You have changed your mind and now want to extend your doctoral studies and to pursue an academic career.

- You are worried that your internship duties will take time away from your dissertation research

Tasks

- Write questions that you plan to ask the director of graduate studies.

- Write questions that you think the graduate students director will ask, and your answers.

Director of Graduate Studies:

You are the new director of graduate studies for your department, and you are about to meet a doctoral student whom you do not know well for a routine annual progress check. From the student's dossier, you see the student started doctoral study five years ago and yet does not seem close to completing the dissertation. The dean of the graduate school and the chair of your department have told you that that the average time to the doctoral degree for students in your department is unacceptably high. These administrators are also concerned that so many graduate students leave the department for industrial positions before they complete their doctoral degrees. Your jobs are to reduce the time to degree and to improve the completion rate.

You see that the student's current research adviser is an eminent professor with rock-star status. This professor's research has received international acclaim, and the professor's company has contributed to the economic growth of the town. Your university strongly supports commercialization of the research of faculty members because of the potential for revenue from royalties. The university also sees local companies as excellent sources of funding and internships for both undergraduate and graduate students.

While you agree that graduate students can benefit from professional internships, you are concerned about two potential ethical problems. First, conflicts of interest can arise when students work at their advisers' companies. In these cases, your department typically appoints a co-adviser without a conflict of interest. Second, students seem ignorant about intellectual property rules. In the past, graduate students have removed notebooks from research laboratories in your department.

Prepare for the annual progress check meeting with the doctoral student.

Summary

- The university strongly supports companies started by professors to commercialize their research
- The graduate dean and your department chair are concerned about time to degree and completion rates
- You are concerned about managing conflicts of interest when students work at their advisor's companies
- You are also concerned that students don't understand how to handle intellectual property

Tasks

- Write questions that you will ask the doctoral student
- Write questions that you think the student will ask, and your answers

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