Letter from New Editor in Chief of Computers and Mathematics with Applications

1 New Aims and Scope of the Journal

The purpose of this letter is to introduce myself and new managing editors of the journal to readers and potential contributors of *Computers and Mathematics with Applications* (CMA).

Upon receiving a proposition from Bob Ross at Elsevier to take over CMA, it became clear to me that I could stand up to the challenge only upon redefining the scope of the journal in such a way that it fits my area of expertise. In short, I am a mathematician and engineer. But I have also worked in a software company, and have spent 30 years developing Finite Element (FE) software. Finally, throughout my 35 year teaching career, I taught a large number of different courses ranging from real and functional analysis, applied mathematics, numerical analysis, various courses in mechanics and engineering and mathematical modeling, to FE software development and coding (see http://users.ices.utexas.edu/ ˜ leszek/) for my current CV). If you are desperate to put a single label on me then the one of a *numerical analyst* would probably be the best fit but also a great simplification.

The redefined CMA will focus on areas contributing to building successful simulations for science and engineering: modeling, analysis and PDEs, discretization methods and numerical analysis, fast numerical algorithms reflecting ever evolving hardware, data structures, software design, code verification and quality assurance (QA) and, finally, Verification and Validation (V&V) in its entire generality.

We expect each new contribution to *clearly indicate* the *goal of the overall simulation effort* and discuss how the presented work contributes to that goal.

Modeling

One could possibly argue that, in modern terms, the entire science as we know, is about modeling different physical phenomena. Starting with Newton's mechanics, development of

- analytical and rigid body mechanics (Euler, Lagrange, Hamilton),
- foundations of continuum mechanics (Cauchy, Cosserats, Piola),
- thermodynamics (Rankine, Clausius, Lord Kelvin, Maxwell, Boltzmann, Planck, Clausius, Gibbs),
- electromagnetism (Coulomb, Ampère, Faraday, Maxwell),
- quantum mechanics (Bohr, Heisenberg, Planck, de Broglie, Einstein, Schrödinger, Born, von Neumann, Dirac, Pauli, Hilbert),
- special and general relativity (Einstein), etc.

and various phenomenological theories developed in 20th century, models expressed in terms of (predominantly) Partial Differential Equations (PDEs) have been developed to face experimental evidence and explain physical reality. Engineering and science have used the models for *prediction* and *design*. Simple models were developed directly (e.g. various beam, plate and shells theories used in structural mechanics), or by means of a more rigorous dimensional reduction leading to various concepts of modeling errors. The last two decades witnessed an explosion of multiscale modeling either through upscaling (e.g. homogenization) or direct linking across scales.

In the end, for a model to be useful, we expect a certain degree of completeness. For PDEs, this includes access to material data, specification of boundary and initial conditions etc.

Traditional areas of modeling in physics and engineering expand rapidly into biology, chemistry, medicine, social sciences. Areas of applications grow but requirements for rigorous mathematics, starting with consistency and stability analysis, remain.

Analysis and PDEs

Once a model has been completed, it becomes a subject of mathematical analysis. Proofs of well-posedness, stability and regularity analysis and derivation of various properties, contribute to the understanding of the model, and frequently help to rectify its logical and mathematical deficiencies. Ideally, we should not proceed with discretization and code development, until the model has been proved to be well posed. In practice, this rarely happens, and we have to be content with sanity checks; formulation and analysis of various *model problems*.

Discretization and Numerical Analysis

Ordinary and Partial Differential Equations (ODEs, PDEs) have to be discretized, i.e. turned into linear and nonlinear algebraic equations that can be solved (approximately) on a computer. This can be done directly (classical Finite Difference (FD) and Finite Volume (FV) methods), through various weak formulations (Finite Element (FE) methods), or through formulation and discretization of equivalent volume or boundary integral equations (Volume and Boundary Element (BE) methods). The discretization process has to be stable and it must converge. Construction of stable discretization schemes and proofs of their convergence is the subject of Numerical Analysis.

Numerical Linear and Nonlinear Algebra. Fast Algorithms

We welcome all work on effective solution of linear and nonlinear systems of equations: iterative methods, preconditioning, multigrid solvers, domain decomposition methods are classical examples of such techniques. Fast algorithms like fast Boundary and Volume Integral methods, Fast Fourier Transform (FFT) - based techniques, and various semi-analytical schemes utilizing e.g. special functions, will remain of interest for the journal.

Algorithms and Data Structures. Adaptivity. Geometry

Having worked myself for over 25 years on various adaptive FE methods, I would like to promote work on adaptivity. Implementation of increasingly more sophisticated numerical algorithms within constantly evolving computer platforms, calls for a continued research in data structures (especially in context of parallel computing) and data structure supporting algorithms. Many successful local refinement techniques still lack proofs of robustness (avoiding "deadlocks", i.e. situations in which mesh refinements cannot be continued due to inefficiency of implemented data structures and algorithms). Finally, although we do not intend to specialize in computational geometry, we welcome all contributions describing interfacing (and integration) with Computer Aided Geometry (CAD), e.g. mesh generation, support of evolving geometry and topology during simulations etc. Finally, innovative scientific visualization techniques (e.g. for higher order methods), remain within our interest as well.

Software Design, Code Verification and Quality Assurance (QA)

Designing and maintaining increasing more complex software is becoming a critical issue. Generality (one program for many problems) is always at odds with efficiency, and the most efficient codes are usually highly specialized and integrated. Code verification (e.g. use of manufactured solutions), self-checking algorithms and QA are important components of successful computer implementations.

Verification and Validation (V&V)

Before a software can be used for *predictions*, it must be verified and validated. Verification deals with control of discretization error, convergence error of iterative algorithms (e.g. linear and non-linear equations solvers), and round-off errors. *A priori-* and *a-posteriori* convergence analysis are typical tools. Validation addresses the quality of models and must be done through comparison with experiments. Material data must be accessed through *calibration* and solution of *inverse problems* of various levels of complexity. Bayesian statistics is perhaps the most popular approach to design the V&V procedures in a systematic way.

Examples of Applications

We welcome contributions presenting applications of the entire simulation process to practical problems in science and industrial engineering. We are especially interested in interdisciplinary problems crossing the traditional boundaries and stimulating new developments. Examples of successful simulation efforts are always very motivating but we also encourage examples of paradoxes, inconsistencies, challenges and open problems in existing theories.

2 Focus and Criteria for Selection

The redefined journal CMA will provide a forum for scientists, engineers and mathematicians involved in computer simulations of physical and engineering processes to present new and important contributions to their field. The

concept of the proposed focus is illustrated in Fig.1.

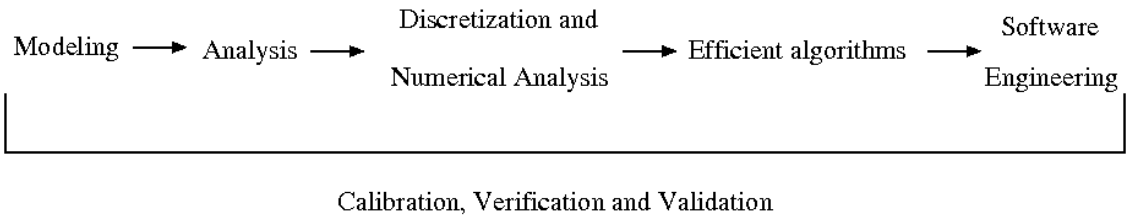

Figure 1: Logical structure of a simulation project

The new journal welcomes contributions to the all outlined fields with one important comment: *The authors have to clearly identify the ultimate simulation effort that proves and illustrates the relevance of their work*. A preference will be give to comprehensive papers (20-30 pages long). We are *not* interested in short notes.

3 Necessary Conditions for Starting the Review Process

Additional necessary conditions for starting the review process include:

- a clear statement *in the abstract* what are the *new* contributions of the paper and in which of the fields outlined above,
- decent English,
- providing a list of 5-7 (the more, the better) potential reviewers that excludes colleagues from the same institution and recent co-authors.

4 Communications

All members of the Editorial Board have the right to accelerate the publishing process and *communicate* directly papers for publications. It is implicitly assumed that the communicating person is either familiar with the work personally or has already performed a review process. The name of the communicating person *will appear* on the published paper.

5 Special Issues

We intend to publish a small number of special issues per year. These do not intend to serve as conference proceedings although they frequently follow organization of specialized workshops or conferences. Those interested in being a Guest Editor of a Special Issue, are invited to send a short proposal along with a CV to the Editor in Chief.

6 Managing Editors

In my editorial work, I will be aided by four colleagues, the *Managing Editors* of the journal: Daniele Boffi from University of Pavia, Italy, Alexander Düster from Hamburg University of Technology, Germany, Jay Gopalakrishnan from Portland State University, USA, and Waldemar Rachowicz from Cracow University of Technology, Poland. Two of them are mathematicians and two are engineers. We follow with short personal introductions from each of them.

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I am a mathematician grown up in Pavia, where my education has been greatly influenced by fruitful interactions with outstanding numerical and mathematical analysts. My primary research field is the finite element approximation of partial differential equations arising from several engineering and biological applications. In this framework, I focused on the analysis of basic properties of finite elements, with particular emphasis on mixed schemes and eigenvalue problems; applications range from fluid-dynamics to electromagnetism. Another important and attractive research interest is related to the numerical approximation of fluid-structure interactions with potential applications ranging from biology to structural mechanics. My teaching experience reflects my scientific background: I am teaching basic numerical analysis and mixed finite elements to mathematicians and basic calculus to biologists. My teaching experience includes Ph.D. courses and summer schools, where I covered eigenvalue approximation and mixed methods.

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With a background in mechanical engineering, my research interests and teaching activities have been focused

on numerical methods with application to engineering problems. My main field of research so far has been devoted to developing finite element methods for nonlinear problems in mechanics. Fields of application range from adaptive, high-order finite element formulations for plates and shells to fictitious domain methods, finite strain problems, computational homogenization methods, multiscale methods and coupled multifield problems. I have taught several courses in linear and nonlinear structural analysis, computational structural dynamics, finite element methods and numerical algorithms, including software development. Summarizing, both my research and teaching are related to computational engineering with the key focus on computational mechanics.

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I am a numerical analyst by training. My research attitudes are shaped by the continuing remarkable successes of algorithms founded on sound mathematical principles. Specifically, I am interested in analyzing and developing new algorithms for numerically solving partial differential equations modeling various physical phenomena. A large portion of my work is concentrated on finite elements, discontinuous Galerkin methods, and multigrid techniques. But I have also enjoyed my interdisciplinary excursions into biological and electromagnetic applications. I often teach courses on the mathematical aspects of finite elements and iterative techniques wherein I take pleasure in bringing the students to the research frontiers.

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My education includes civil engineering and physics. I taught various kinds of mechanics (structural mechanics, strength of materials, linear and nonlinear elasticity), numerical methods (including Finite Element Method and adaptive methods), calculus and linear algebra.

My main research interests are in adaptive Finite Element methods. I have worked on adaptive FE methods in the following areas: elliptic problems (including structural mechanics), computational fluid dynamics, computational electromagnetics and acoustics, inverse scattering problems and biomechanics.

7 New Editorial Board

I sincerely thank all members of the old Editorial Board for their dedicated service and help in running the journal, many from the very beginning of its creation by the Founding Editor - Prof. Ervin Rodin. Due to the redefined scope and aims of the journal and the new editorial crew, we have decided to restart the Editorial Board as well by inviting new members whose research corresponds and reflects the new goals of the journal.

I would like to finish by thanking Dr. Rodin for nominating me for the Editor–in–Chief position, and Bob Ross and Elsevier for their trust. I hope that along with the Managing Editors and the new members of the Editorial Board, I will be able to meet the expectations of our communities and serve the needs for a quality and timely publishing in our fields.

Sincerely yours,

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