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「第３の科学
～計算力学がもたらす科学技術革新～」

テキサス大学オースティン校計算工学・科学研究所（ICES）設立所長、教授

ティンズリー・オーデン博士

THE THIRD PILLAR: The Computational Revolution of Science and Engineering

Commemorative lecture at the 34th Honda Prize
Award Ceremony on the 18th November 2013

Dr. J. Tinsley Oden

Ph.D., Founding Director of the Institute for Computational Engineering and Sciences (ICES), The University of Texas at Austin

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Dr. J. Tinsley Oden

■生まれ

1936年12月25日	ルイジアナ州アレクサンドリア生 (アメリカ国籍)

■学　歴

1959年	ルイジアナ州立大学土木工学科卒業
1960年	オクラホマ州立大学土木工学科修士課程修了
1962年	オクラホマ州立大学機械工学科博士課程修了

■名誉学位

1987年	ポルトガル・リスボン工科大学より 名誉博士号
2000年	ベルギー・モン理工科大学より 名誉博士号
2001年	ポーランド・クラクフ工業大学より 名誉博士号
2004年	テキサス大学オースティン校にて 学長表彰
2006年	フランス・カシャン高等師範学校より 名誉博士号
2010年	オハイオ州立大学より名誉博士号

■職　歴

1959年	ルイジアナ州立大学助手
1961年～63年	オクラホマ州立大学応用力学科講師、 土木工学科准教授
1963年～64年	General Dynamics 社勤務 (研究部門構造担当シニア技師)
1964年9月 ～73年８月	アラバマ大学ハンツビル校 機械工学科 助教授～教授
1973年9月 ～現在	テキサス大学オースティン校 航空宇宙工学/機械工学科教授
1974年9月 ～現在	テキサス大学オースティン校 計算工学・科学研究所(ICES)所長 (1974-1993 TICOM, 1993-2003 TICAM)
1981年9月 ～現在	テキサス大学オースティン校 数学科教授
2003年3月 ～現在	テキサス大学オースティン校 研究担当副校長
2011年～現在	テキサス大学オースティン校 コンピューター科学科教授

■BORN

December 25, 1936 in Alexandria, Louisiana, USA
(USA citizenship)

■EDUCATION AND TRAINING

1962	Ph.D., Oklahoma State University, Engineering Mechanics
1960	M.S., Oklahoma State University, Civil Engineering
1959	B.S., Louisiana State University, Civil Engineering

■HONORARY DEGREES

2010	Ohio State University Honoris Causa
2006	Ecole Normale Superieure Cachan (ENSC), France Honoris Causa
2004	The University of Texas at Austin Presidential Citation
2001	Cracow University of Technology, Poland Honoris Causa
2000	Faculte Polytechnique de Mons, Mons Belgium Honoris Causa
1987	Technical University of Lisbon, Lisbon, Portugal Honoris Causa

■EMPLOYMENT HISTORY

University of Texas-Austin, Director, Institute for Computational Engineering and Sciences (ICES), (TICOM 9/1974 - 8/1993, TICAM 9/1993 - 2/2003) 3/2003 - present.

University of Texas-Austin, Associate Vice President for Research, 3/2003 - present.

University of Texas-Austin, Professor, Computer Science Department, 2011 - present.

University of Texas-Austin, Professor, Mathematics Department, 9/1981 - present.

University of Texas-Austin, Professor, Aerospace Engineering and Engineering Mechanics Department, 9/1973 - present.

University of Alabama-Huntsville, Assistant Professor and Professor in Engineering Mechanics, 9/1964 - 8/1973.

General Dynamics, Senior Structures Engineer, Research Department, Fort Worth, 1963-64.

Oklahoma State University, Instructor in Applied Mechanics, Assistant Professor in Civil Engineering, 1961 - 63.

Louisiana State University, Teaching Assistant, 1959.

■略　歴

オーデン博士は工学、数学、そしてコンピューター科学を統合し、自然科学の世界にコンピューター・シミュレーションを生み出した、計算力学の創設と発展に多大な貢献をしたことで国際的な名声を得ている。このようなシミュレーションは、医学、材料工学、エネルギー探査そして気候科学など様々な分野で活用されている。現在博士はテキサス大学オースティン校において計算工学・科学研究所所長として、半導体モデルと癌治療に主眼を置いたマルチスケール“アダプティブ”モデルの研究を進めている。また、アメリカ土木学会のカルマンメダル(1992年)、アメリカ計算力学学会のニュウマンメダル(1993年)、国際計算力学連合のニュートン・ガウスメダル(1994年)、アメリカ機械学会のティモシェンコメダル(1996年)他多数を受賞している。

■出版物

“Mechanics of Elastic Structures”：
McGraw-Hill, New York City, 1967年

“非線形連続体の有限要素法”：
McGraw-Hill, New York City, 1972年

“Finite Elements vol.1 to 6”：
(E.B Becker および Graham F. Carey 共著)
Prentice-Hall, Englewood Cliffs, 1981年

“Applied Functional Analysis, 2nd ed.”：
(L. F. Demkowicz 共著)
CRC Press, Boca-Raton, 2010年

“An Introduction to Mathematical Modelling”：
Wiley, Hoboken, 2011年

(27冊の著作を含め、800にも及ぶ論文、記事の中から抜粋)

■BIOGRAPHICAL SKETCH

J. Tinsley Oden is world renowned for his contributions in establishing and developing the field of computational mechanics, which applies mechanics, mathematics, and computer science to create computer models of the physical world. Such simulations are used in fields as diverse as medicine, material engineering, energy exploration, and climate science. As the Director of the Institute for Computational Engineering and Sciences, Dr. Oden's current research is in multi-scale “adaptive” modelling, with a focus on semiconductor modelling and cancer treatment. For his scientific contributions, Dr. Oden was awarded the Theodore von Karman Medal of American Society for Civil Engineers in Engineering Mechanics in 1992, the John von Neumann Medal of U.S. Association for Computational Mechanics in 1993, the Newton-Gauss Congress Medal of International Association for Computational Mechanics in 1994, and The Stephen P. Timoshenko Medal of American Society of Mechanical Engineers in Applied Mechanics in 1996, among others.

■PUBLICATIONS

Mechanics of Elastic Structures：
McGraw-Hill, New York City, 1967

Finite Elements of Nonlinear Continua：
McGraw-Hill, New York City, 1972

Finite Elements vol.1 to 6：
(with E.B Becker and Graham F. Carey)
Prentice-Hall, Englewood Cliffs, 1981

Applied Functional Analysis, 2nd ed.：
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CRC Press, Boca-Raton, 2010

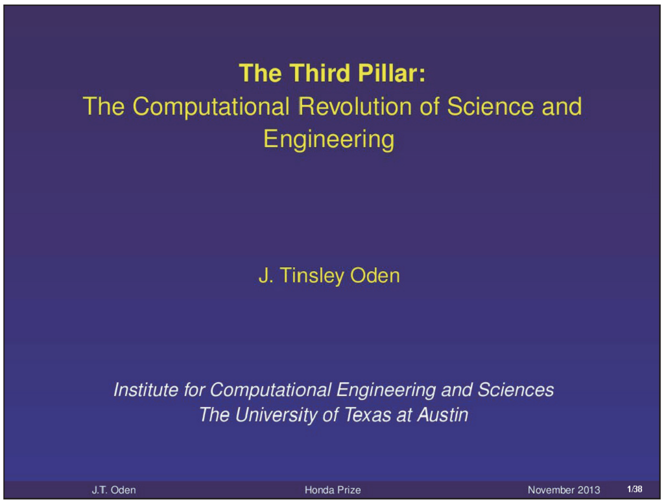
An Introduction to Mathematical Modelling：
Wiley, Hoboken, 2011

(selected among 800 publications, including 27 books)

このレポートは、2013 年 11 月 18 日　東京、帝国ホテルにおいて行なわれた第 34 回本田賞授与式記念講演の要旨をまとめたものです。
This report is the gist of the commemorative lecture at the 34th Honda Prize Award Ceremony at the Imperial Hotel, Tokyo on 18th November 2013.

THE THIRD PILLAR:
The Computational Revolution of Science and Engineering

J. Tinsley Oden



I am truly humbled by this great honor bestowed on me by the Honda Foundation. This extraordinary ceremony, the participation of such distinguished guests, and the honor of being included as part of the great tradition of the Honda Prize represent events marking the peak of one's professional life. This is truly the high point of my career as a computational scientist, an engineer, a mathematician, and a researcher. I give my sincere thanks to the Honda Foundation, Mr. Hiroto Ishida, President of the Honda Foundation and to the selection committee for kindly selecting me and my work for this award. I convey my sincere appreciation to Mr. Fumihiko Ike, Chairman and Representative of the Honda Motor Company, Ltd. I also thank other distinguished guests who took the time to attend this ceremony and share with me this special event. I am particularly grateful to Mr. Satoshi Matsuzawa, Managing Director of the Honda Foundation, whose kindness and professional assistance made this occasion all the more enjoyable. And I thank my dear friends here who have interacted with me professionally and socially over the years who are part of my most respected supporters. Thank you all for attending this ceremony.

I also embrace the ecotechnology concept of the Honda Foundation, and hope to lay down arguments that computational mechanics—and more broadly, computational science—has had, and will continue to have, a profound impact on all of science and technology, and will emerge as an indispensable factor in preserving our precious ecological systems and advancing ecotechnologies in the future.

I am indebted to many individuals who supported me and my work on the long path that brought me to this point in my life: my family, my wife Barbara, son Walker, and daughter Lee, who patiently and lovingly sacrificed time with me so I could do my work; to my parents, who encouraged me as a child and an adult to devote myself to scholarship and research; and to many students, postdocs, and professional colleagues, some of whom are here at this ceremony, who collaborated and supported much of my work over the years.

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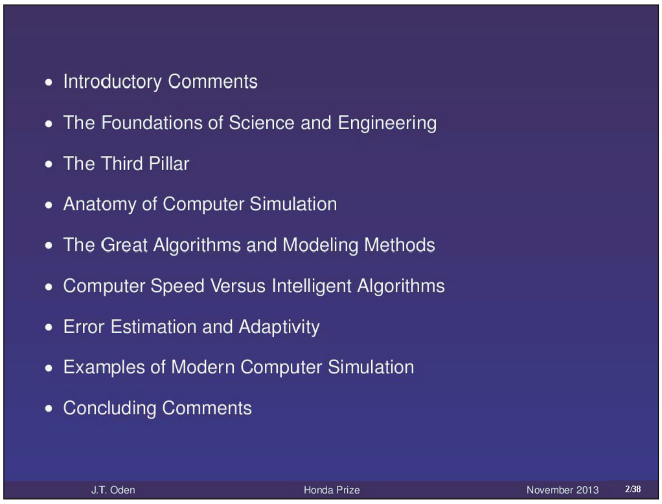

Fig 1

〈Fig 1〉 This presentation is divided into the nine topics indicated here, beginning with the introductory comments I make now.

■ Foundations of Science and Engineering

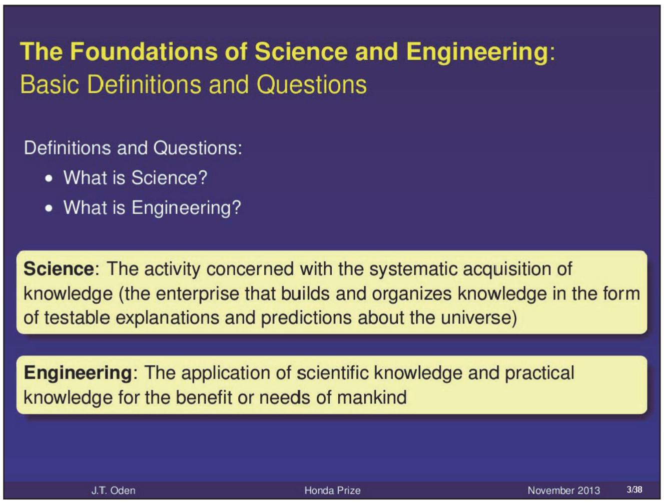

Fig 2

〈Fig 2〉　I begin this lecture with a few comments on ancient subjects of concern to all of us here: *science*, the *scientific method*, and its application to problems affecting mankind. A simple definition of science is this: *the activity concerned with the systematic acquisition of knowledge.* The English word is derived from *scientia*, which is Latin for “knowledge.” According to the Cambridge Dictionary, it is “the enterprise that builds and organizes knowledge in the form of testable explanations and predictions about the universe.” It is designed to reduce or eliminate ignorance by acquiring and understanding information and involves the mental comprehension of perceived truth or fact through cognition. Engineering is the systematic application of scientific and practical knowledge for the benefit or needs of mankind.

Few doubt the importance of scientific discoveries and the enormous advances they have made possible in technology over the last millennium in improving the welfare, safety, longevity, and richness of life of the human species. With advances in science, comes understanding of the universe in which we live, the forces and laws that govern it, and ultimately the ability to control those forces and direct them in a way to benefit humankind.

I believe that to dedicate one’s time and energy to science, that is, to acquire knowledge, and more importantly to apply it, is one of the most honorable activities in which one can engage, but, it is also an activity that is enormously challenging, and, at the same time, remarkably exhilarating.

■ An Ancient Question and Debate

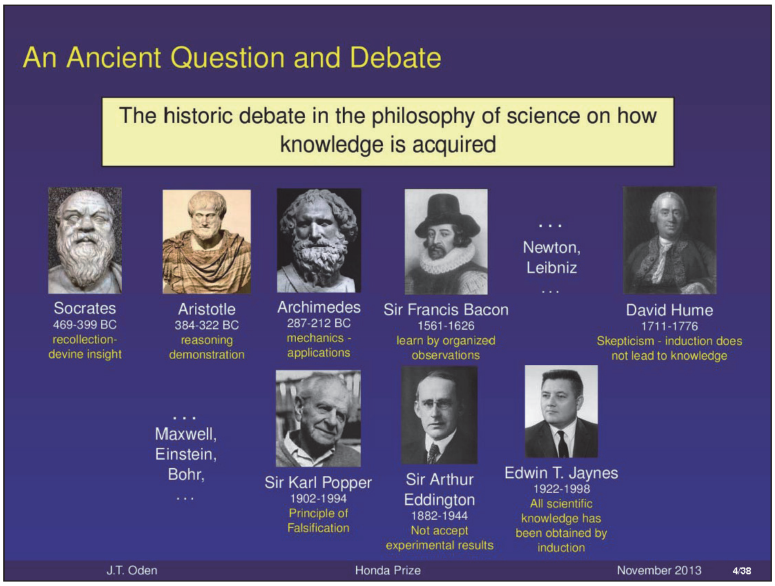

Fig 3

〈Fig 3〉 The question of how knowledge is acquired has been a subject of debate among philosophers of science for almost 3,000 years. We find, from the writings of Plato on Socrates, the great philosopher who lived between 469-399 BC, that Socrates believed that knowledge lies in the immortal soul. Not trusting the human senses, he believed that knowledge occurs by recollection or divine insight, and Plato, his student, aggressively perpetuated that thinking. But Plato's student, Aristotle, who lived between 384–322 BC, had a more appealing answer: knowledge is acquired by reasoning and demonstration—a precursor to the idea that physical observation and inductive hypothesis create knowledge. In the two millennia between 500 BC and the 15th century, we had the likes of Archimedes, da Vinci, and others. Sir Francis Bacon, David Hume, Galileo, Newton, and others followed in the 16^{th}-18^{th} centuries, and then, in the 20^{th} century, there was Dirac, Eddington, Bohr, Einstein, Maxwell, Boltzmann, and many more.

Sir Francis Bacon, who is credited with influencing the dawn of the industrial age, put forth the idea that everything is learned by induction and organized observations. This notion was addressed by the British philosopher David Hume, who founded the philosophy of skepticism, based on the proposition that induction cannot lead to knowledge. Knowledge, according to Hume, can only be obtained through observation and experiment. By induction, we mean the development of hypotheses, generally theories, based on interpretations of causes of observations of physical events, and, then extrapolating from those hypotheses to forecast future events, or events in the past.

Ultimately, the great scientists of the 19th and 20th centuries, ignoring or oblivious to the pessimism of Hume, continued to develop inductive theories that changed the world. But the philosophical foundations were still unsettled until the work of Karl Popper, the 20th century philosopher, who put forth his principle of falsification, to wit: an inductive hypothesis, a theory, cannot qualify as a true scientific theory unless it were possible to falsify it through observations contrary to predictions; that is, unless it were possible to acquire observations that could be in conflict with the theory. Without the possibility of falsification, the hypotheses were pseudo-science and not a true scientific theory. Once falsified, the theory could be modified to agree with observations or discarded. And so we came to recognize that a scientific theory, a product of induction, is only valid as long as it is not contradicted by physical observations. A mathematical theory, on the other hand, which arises from deductive reasoning (the establishment of axioms and then using mathematical logic to prove the consequences of those axioms) is permanent and unfailing, and does not change. Thus, correct mathematical proofs last forever; scientific proofs last only until they are contradicted by observations. Even Popper was eventually criticized as being too objective. It was said that the philosophy of objectivism was not how real science was done. Real observations of the physical universe account for the statistical nature of events, and Popper's principles, at least early versions of them, did not use statistical interpretations.

As the 20th century progressed, we came across the likes of extraordinary scientists who made inductive contributions to what we know about the physical universe: Rene de Broglie formalized the relationship between electromagnetic waves and momenta a decade before these relationships were confirmed experimentally. Also, Paul Dirac, purely on the basis of mathematical calculations, discovered the existence of anti-matter, a physical reality that was only observed experimentally a dozen years after his announcement. This led Sir Arthur Eddington, who confirmed Einstein's theory of relativity through astronomical observations long after they had been predicted by the theory of relativity, to comment, "the experimentalist will be surprised to learn that we will not accept experimental data unless it is confirmed by theory". This was clearly opposite to the views of Hume and others. More recently, the physicist and probabilist, Edwin T. Jaynes, put forth the notion that all science is inductive, that an inductive process must be used, even when one wishes to design experiments, or to assimilate and mine data, or to explain the causes of events observed in existing physical systems.

■ The Classical Pillars of Science

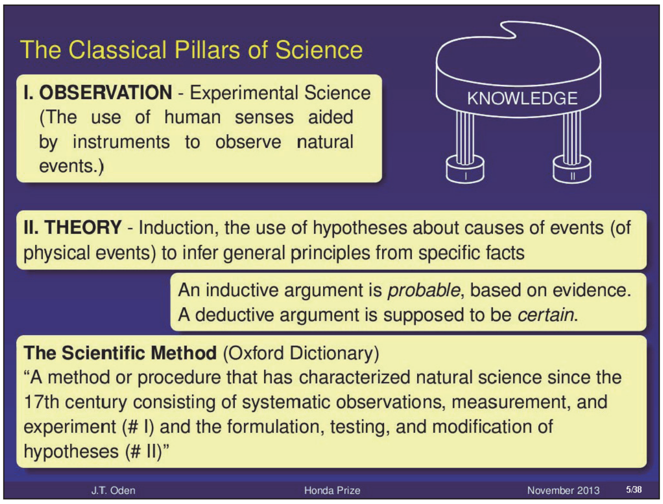

Fig 4

〈Fig 4〉 Thus, after millennia of debate by the greatest minds of human history, two avenues to scientific knowledge emerged: 1) observations, experimental measurements, information gained by the human senses, guided by instruments, and 2) theory, inductive hypotheses often framed in mathematical language. Observation and theory are thus, the two classical pillars of science. According to the Oxford Dictionary, the scientific method is "a method of procedure that has characterized natural science since the 17th century, consisting in systematic observation, measurement, experience and experiment and the formulation, testing, and modification of hypotheses."

■ Is There a Third Pillar?

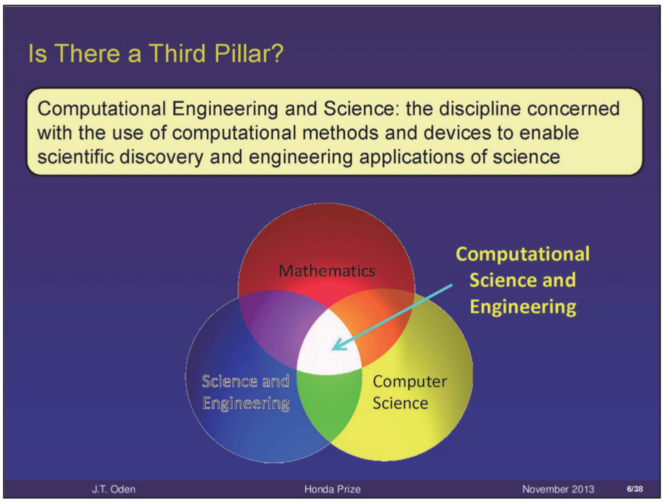

Fig 5

〈Fig 5〉 Is there a third pillar? Is there a new avenue to gain scientific knowledge? The answer, in my mind, and in the minds of most contemporary scientists and engineers, is very clearly "Yes." It is the new discipline of *computational science*: the use of computers and models, computational algorithms, and computing devices to fashion models of how the physical universe behaves to predict the future, and also reconstruct the past. In little more than a half century of the two to four million years of human history or, on a historic scale, in the blink of an eye, the entire scientific landscape has changed forever. Computational science is the most important scientific event in human history. It has transformed forever the way scientific discoveries are made and how engineering applications are performed. It lies at the intersection of mathematics, computer science, and the core disciplines of science and engineering. Mathematics, because it is the language in which scientific theory is written, as well as the language to transcribe and transfer information on observations, is an indispensable component of the classical pillars of science. Mathematics is also the language in which the mathematical theories of science are reconstituted and put in a form that can be processed by digital computers. Computer science is the body of scientific knowledge and technology designed to understand and build computing devices, and to develop the language and means to communicate with computing machines. Of course, the traditional core disciplines of science and engineering must now be reviewed and reconstituted because what had once been out of reach by traditional science is now well within reach because of the advent of powerful new tools and approaches afforded by computational science.

Computational science, I submit, is the Third Pillar of Science. It embodies the development of computer models, computer simulations, data retrieval and mining, processing of large data sets, and explicit advances in computing technology. It enables scientific discovery and advances never thought possible before—in manufacturing, medicine, surgery, materials, climate science, geophysics, in understanding natural hazards, and many other areas of technology and scientific study.

■ Mechanics and Computational Mechanics

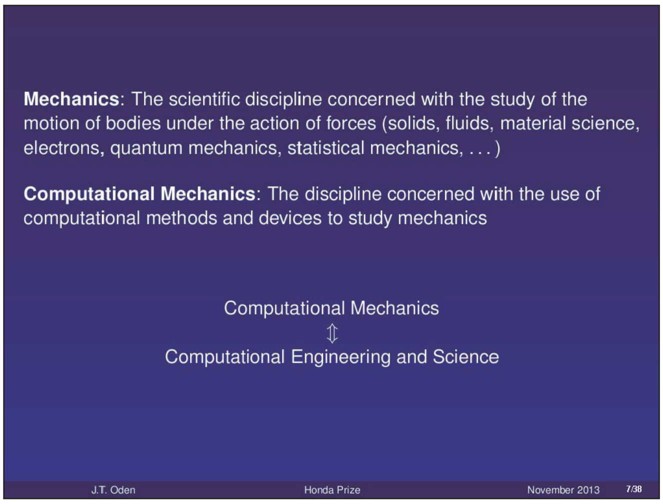

Fig 6

〈Fig 6〉 My introduction to this subject began by studying mechanics and computational mechanics, the scientific discipline concerned with the study of the motion of bodies under the action of forces; so it embraces solid mechanics, fluid mechanics, but now also includes materials science, the motion of electrons, quantum mechanics, and statistical mechanics. In my mind, with a clear, broad definition of mechanics, it is indistinguishable from computational science.

■ What can CSE do that classical science cannot?

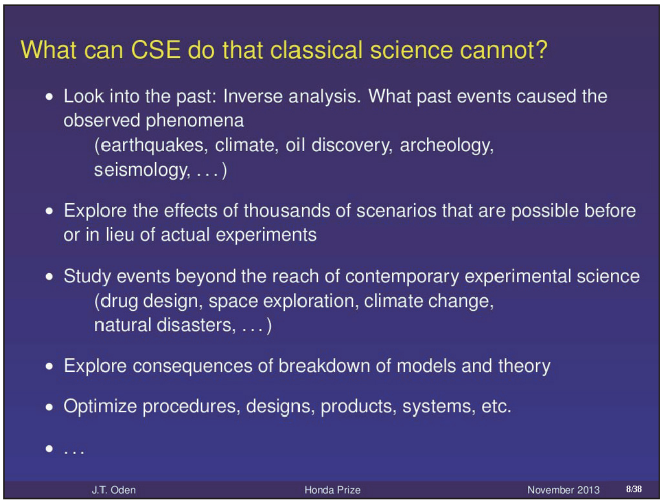

Fig 7

〈Fig 7〉 What can computational science and engineering do that classical science cannot? It can look into the past with inverse analysis, to determine what past events caused observed phenomena. It can explore the effects of thousands of scenarios for or in lieu of actual experiments. It can be used to study events beyond the reach of expanding the boundaries of contemporary experimental science, such as in drug design, space exploration, climate change, and natural disasters. It can even explore the consequences of a breakdown in models and theories. It can optimize procedures for the design of projects and systems.

■ The Anatomy of a Computer Simulations

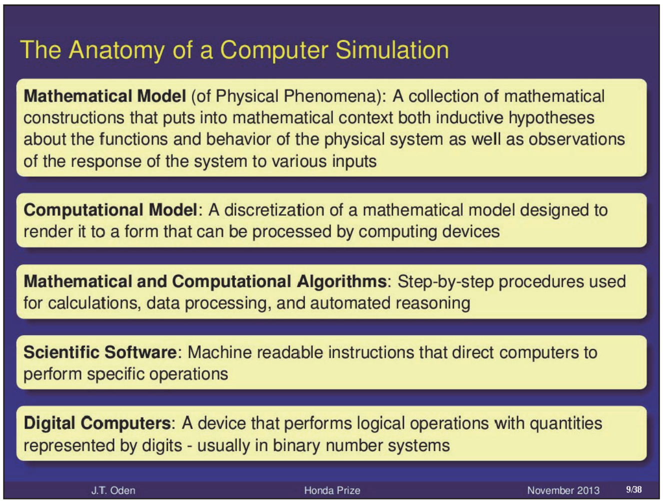

Fig 8

〈Fig 8〉 Let us now dissect the anatomy of a computer simulation. Exactly what is involved in applying the tools of computational science to acquire knowledge or to understand the behavior of engineered systems? First, there is the mathematical model, which is a collection of mathematical constructions that translates both inductive hypotheses about the functions and behavior of the physical system, as well as observations of the response of the system to various inputs within a mathematical context. Second, there is the computational model, a corrupted discretization of the mathematical model rendering into a form that can be processed by computing devices. Third, there are mathematical and computational algorithms that are step-by-step procedures and formulations used for calculation, data processing, and automated reasoning. Fourth, there is scientific software that delivers machine-readable instructions that direct computers to perform specific functions. Then, there is the computer, the device that performs logical operations with quantities represented by digits usually in binary number systems. Finally, there is the output data, which must be processed and interpreted and used in predictions or designs or in decision making.

■ The Anatomy of a Computer Simulation 2

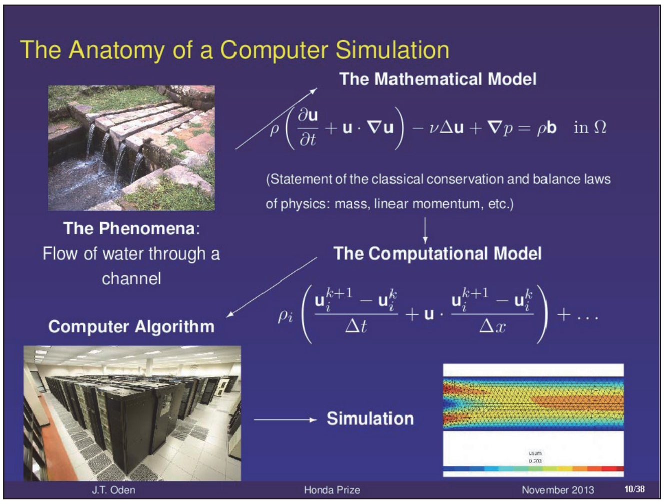

Fig 9

〈Fig 9〉 A good example of a computer model of a physical phenomenon is that of flow of water through a channel. One could assume that the system is governed by the fundamental laws of conservation of mass, and the principles of conservation and balance of linear and angular momentum. Assuming the laws governing the motion of viscous fluids, one chooses the renowned Navier Stokes equations as a mathematical model of the physical phenomenon. For this case, let us select a quantity u for the velocity of the fluid, ρ as its density, ν its viscosity, a physical parameter, p the pressure, and b the body force, such as might be represented by the weight of the fluid or its buoyancy. This is a mathematical characterization of a theory, embodied in the principle of balance of momentum. To render it into a form that can be computed, we discretize it: we replace derivatives of functions with discrete approximations to produce a computational model, and then we develop a code, a computer program, and implement the solving of the computational model on a computer. This produces a discrete characterization of the solution of the model that depicts the fluid flow we originally set out to simulate. There is another step between the production of the computed results and their use, and that is to develop, interpret, and visualize the solution, and to use one's knowledge to infer the behavior of the system. So, once again, the methods and techniques of modern computer science enter the picture.

■ The Greatest Modeling Methods and Algorithms of Modern History Made Possible by Computers

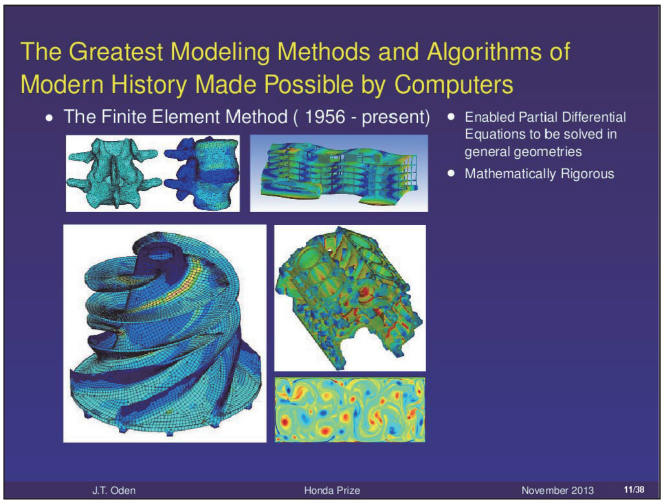

Fig 10

〈Fig 10〉 What are the methods and algorithms of modern history that have made these advances possible? Some modern computational methods would not have existed without the advent of computers. The first I will mention is the finite element method. Generally regarded as having been created in the 1950s, with some vestiges of it going back much further, the finite element method continues to be developed and used extensively today. It is an ingenious method in which a complex physical problem is divided into small pieces, its finite elements, and the laws of mechanics are applied to each individual piece. These are then packed together to form complete models of large, complex systems. The finite element method has impacted virtually every area of science and technology. I had the good fortune to play a role during its early years and to develop some of the earliest computer programs that implemented the method for the analysis of complex aerospace and aeronautical systems. That was in the early 1960's. Later, in the 1970's, I authored one of the earliest books on its mathematical foundations, a subject which has become a rich and active branch of applied and computational mathematics, and is taught worldwide.

■ The Greatest Modeling Methods and Algorithms of Modern History Made Possible by Computers 2

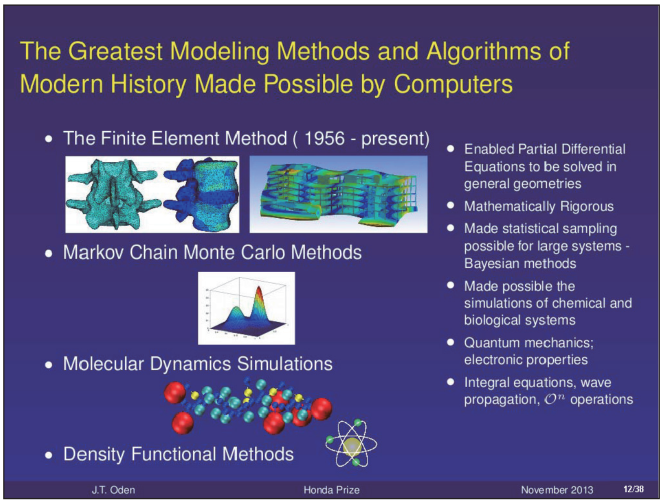

Fig 11

〈Fig 11〉 Basically, the finite element method enabled the engineering and scientific community to solve partial differential equations on geometrically complex domains, and it is mathematically rigorous. Not only did the ability to solve partial differential equations create a huge impact on modern mathematics, but it also revolutionized engineering. Other methods of statistics and statistical sampling are enabled by advances in computers and are manifested in the powerful new algorithms such as the Markov Chain Monte Carlo method, the use of molecular dynamics to the study of chemistry, the study of statistical methods, stochastic systems, and so on. These fields would never have existed had it not been for the advances of digital computing and computational mathematics in the 1980s and 1990s. Now these statistical sampling methods are becoming fundamental tools in many areas of science and engineering. Molecular dynamics simulations are used in biology, in the understanding of the behavior of viruses and bacteria, in the development of nanoparticles for drug delivery, and in engineering new materials. These are computational algorithms that model nature at an atomistic or molecular level. They have had a tremendous impact on how we understand, teach, and use modern biology, chemistry, and physics. Next is the Density Functional Theory, a theory of quantum systems that led to the development of a revolutionary reformulation of quantum mechanics that brought a host of new methods to solve problems at the electronic level and to the study of first principles in the behavior of materials and physical systems. More recently, several new, very fast algorithms have been designed that enable the solution of very large problems with billions of unknowns in a fraction of the time of the methodologies and algorithms that were available back in the 1980s and 1990s. These have led to huge advances in such fields as seismology that help find and exploit vital reserves in oil and gas.

■ Are Advances in Computational Science Strictly Due to Advances in the Size and Speed of Computers?

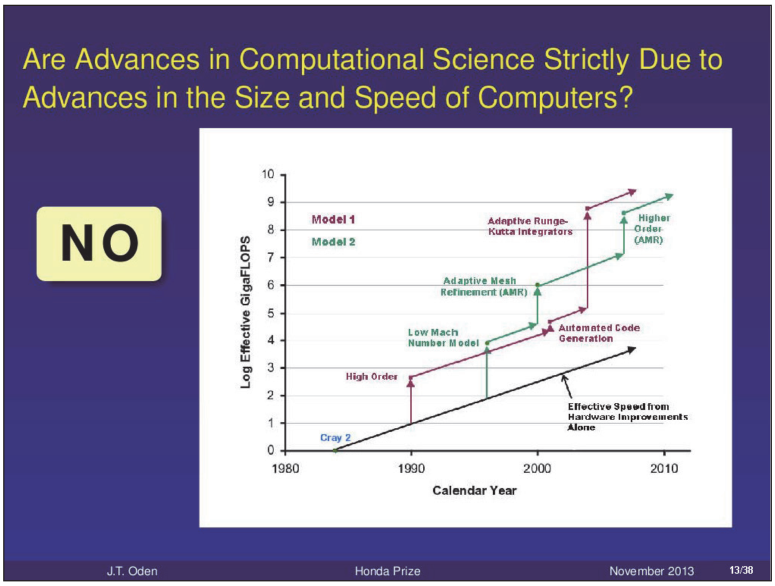

Fig 12

〈Fig 12〉 In viewing these scientific advances brought about by computing, one may ask: can all of these be attributed strictly to advances in the size and speed of computers? I must register emphatically a resounding "No" to this question. Many, many counterexamples can be registered. The graph shown indicates that if one plots the effective gigaflops on a computing device against the calendar year in which advances in computer speeds were made, for example, in proportion to the number of semiconductors per computer chip, this corresponding increase is roughly linear over the last 30 years, a well-known and documented fact. When one factors in great advances in algorithms, many of which have already been mentioned, the effective size, processing speed and complexity of problems, have increased by four orders of magnitude. Computers alone have contributed to only a portion of the advances in computational science in recent years.

■ Imperfect Paths to Knowledge

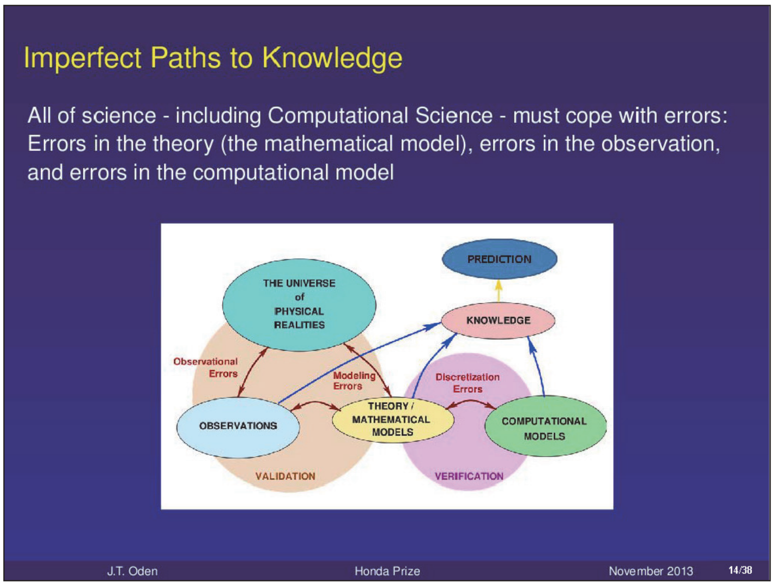

Fig 13

〈Fig 13〉 In modern computational science, every phase of the scientific method involves uncertainty. It is in observations, in data characterizing the models, and in the models themselves, since they are only mathematical abstractions of reality. There is also uncertainty due to the discretization of the model which casts it into a form that can be processed by a computer. The management of all these uncertainties and their quantification and control, using modern methods of statistics and probability, are now at the cutting edge of research in computational science. While the presence of uncertainty in scientific predictions has been recognized for many years, it has only been in recent times that modern algorithms, methods, and computing machines reached the level of development at which significant advances can be made to manage these uncertainties, and to control and quantify them. This is a subject I have been working on steadily over the past decade, and I believe we are close to developing a full and rigorous theory for uncertainty quantification and for creating the foundations of what is called "predictive science."

■ Error Estimation and Adaptivity

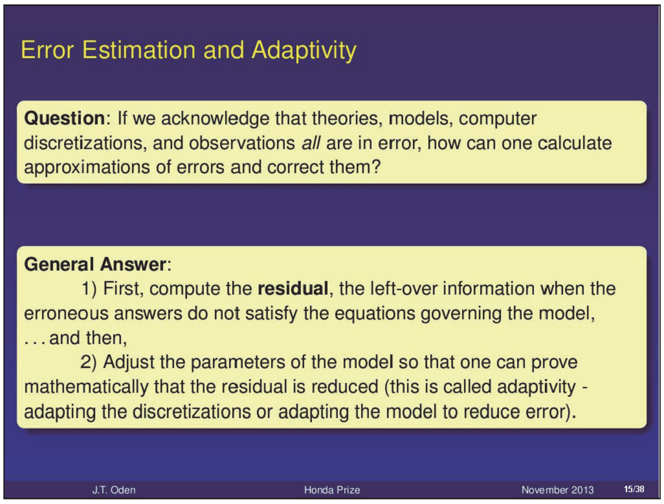

Fig 14

〈Fig 14〉 And, we now turn to an area related to my earlier comments on the fallibility of computers, models, and even scientific theories in predicting the future. In solving complex problems, have we developed over the past decades any way to estimate these errors, to reduce them, and to control them? The answer is "Yes," and, in fact, the whole subject of error estimations and adaptivity is a huge and important area in computational science and one in which I have had the privilege to be involved. The general question is this: if we acknowledge that theories, models, and computer discretizations and observations are in error, how can one calculate approximations of error and correct them? The general answer that I have used in my work is to compute what is called a residual. A residual is leftover information that results when erroneous answers do not satisfy the equations governing the computational model. Then one needs to adjust the parameters of the model so that one can prove mathematically that the residual is reduced. This is called adaptivity, and adapting the discretizations, or adapting the model to reduce error, is a fundamental concept that has permeated much of the modern work in computational science, including my own.

■ The Last Word: The Path to Truth

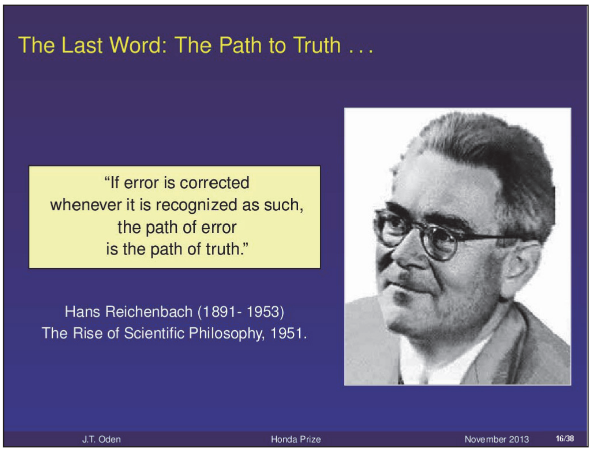

Fig 15

〈Fig 15〉 The philosopher Hans Reichenbach states in his book The Rise of Scientific Philosophy that, "If error is corrected whenever it is recognized as such, the path to error is the path to truth." This is the underlying philosophy of adaptive computational methods.

■ Examples of CS&E Research at ICES

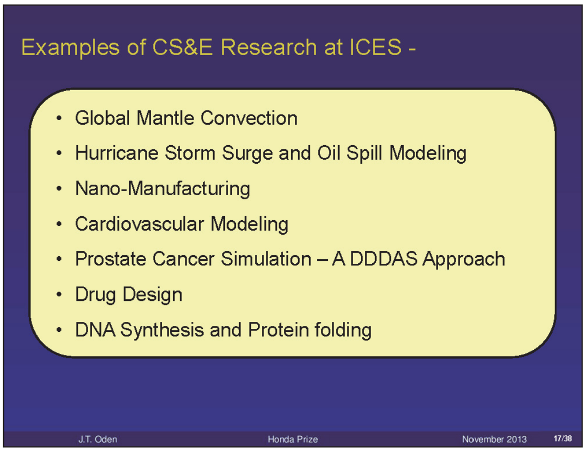

Fig 16

〈Fig 16〉 I would now like to list a few examples of modern applications of computational science that have been performed at my institute over the last half decade.

■ Global Mantle Convection Modeling

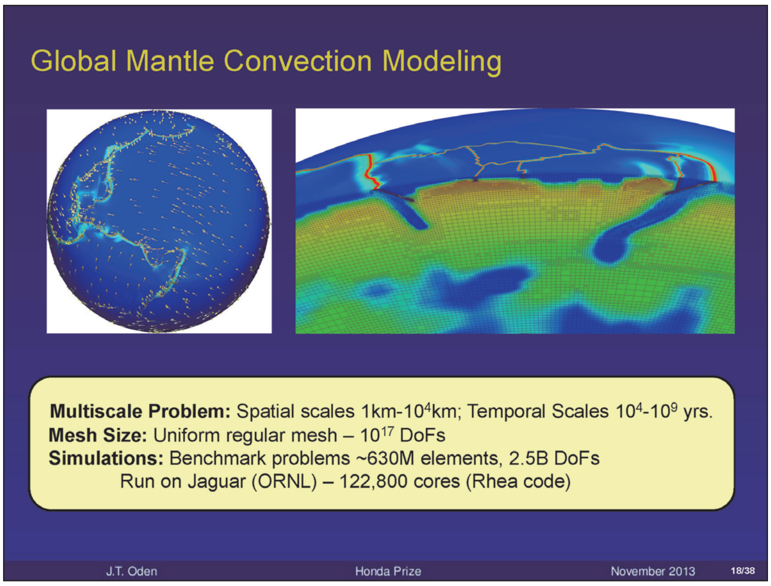

Fig 17

〈Fig 17〉 This example is a remarkable calculation of the cooling of the earth's core and the creation of the earth's mantle, a spherical shell exterior to the core modeled as a viscous creeping incompressible, non-Newtonian fluid. The model involves the fundamental equations of balance of momentum, mass, and energy. It is this model that was featured in *Science Magazine* and, indeed, was on the cover of *Science* in 2010. It pictures a model of around 300 million hexahedral finite elements, around 1.2 billion degrees of freedom, and solved on around 5,000-10,000 processor cores of the Ranger super-computer system. The calculation was done about three years ago by a team at ICES Center for Computational Geosciences and Optimization, led by Omar Ghattas, and took on the order of 100,000 time steps.

■ Mantle Convection Simulation

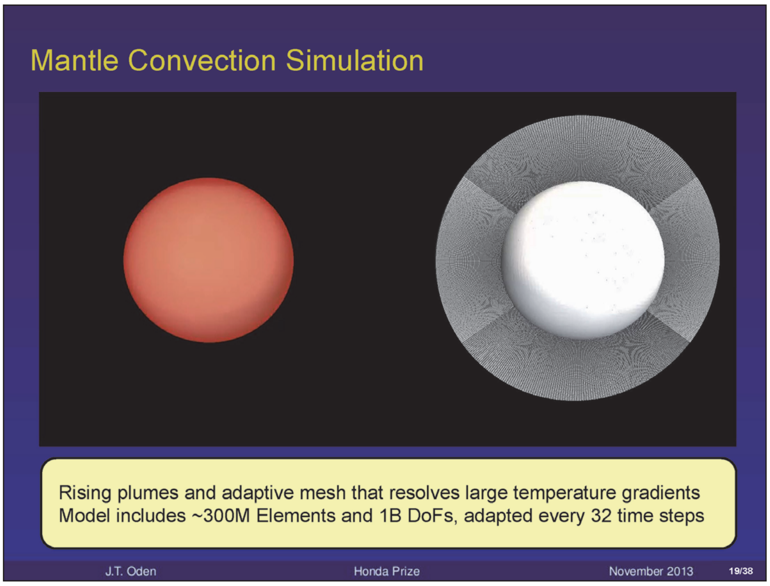

Fig 18

〈Fig 18〉 The movie shows that the Earth's mantle arises from plumes of warm rock flowing buoyantly from the mantle core. The plumes, called upwellings, flow along the earth's crust upward. They subsequently cool and break down back into the core of the earth. These are called downwellings. The round trip of these convection cells is on the order of a few hundred million years, with a typical flow velocity of a few centimeters per year. This phenomena is thought to drive plate motion to the earth's surface in a very high Reynold's number flow, which is very unstable and requires 10 kilometers of resolution of the sharp thermal fronts and even finer one kilometer resolution at the plate boundaries. This resolution would lead to an intractable computation since the earth has an excess of around one trillion cubic kilometers. Adaptive mesh refinement reduces the number of elements needed by a factor of 5,000. The movie also shows that large thermal gradient regions and regions of large viscosity promote dynamically adaptive meshing to control the resolution of important physical details predicted in the model.

Ultimately, predicting the behavior of the complete dynamical system responsible for plate motion and earthquakes, the creation of volcanoes, mountain ranges, and long-term sea levels will fill enormous gaps in our knowledge of questions that are basic to principles of driving and resisting forces of plate tectonics and what is the energy balance of the planet as a whole. The understanding of mantle convection has been designated as one of the Ten Grand Research Questions in Earth science. We are building these models to help answer these questions.

■ Hurricane Storm Surge and Oil Spill Modeling in the Gulf of Mexico

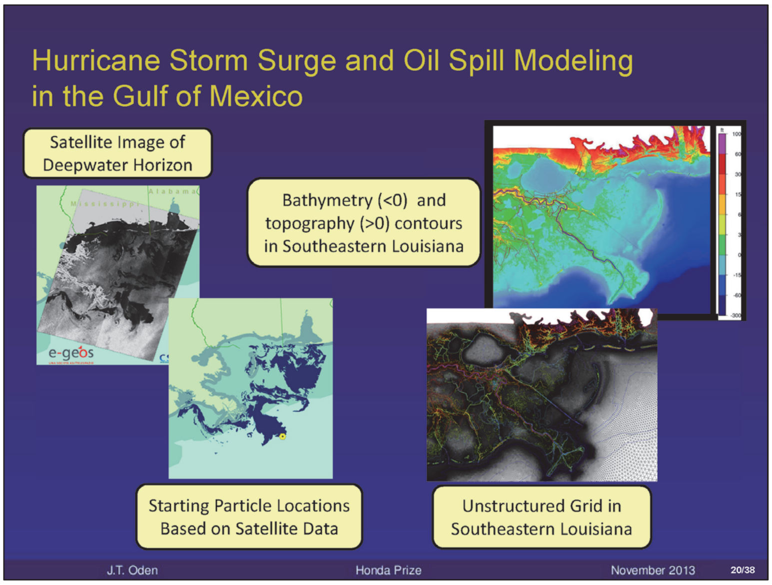

Fig 19

■ Hurricane Storm Surge and Oil Spill Modeling Using the ADCIRC Code

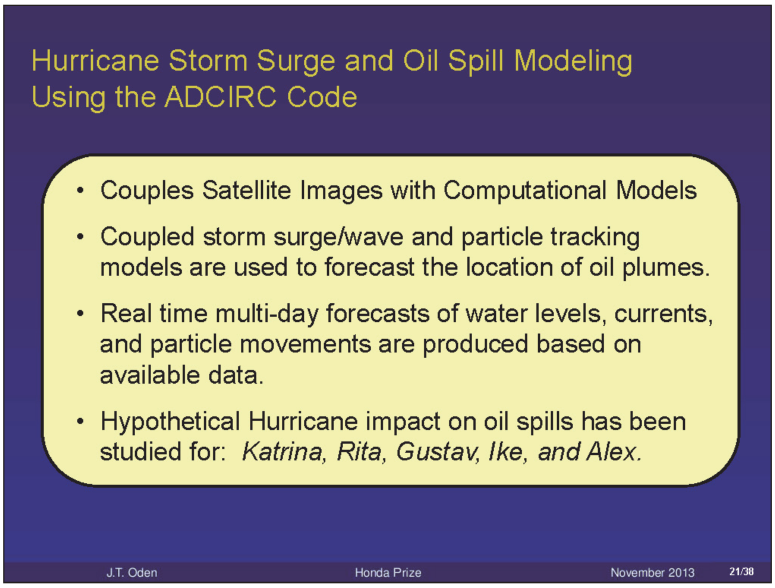

Fig 20

■ **Hurricane Storm Surge and Oil Spill Modeling – Hurricane Katrina and the Deepwater Horizon**

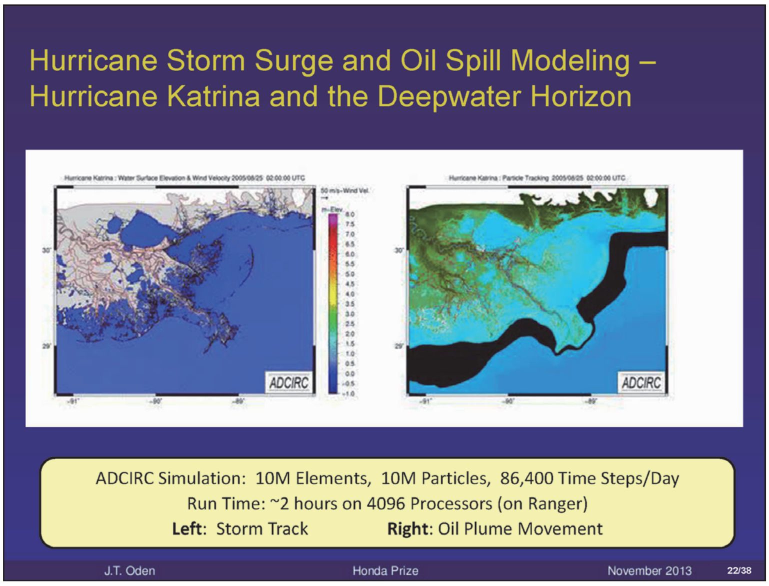

Fig 21

〈Fig 19-21〉 Next, we show the hydrology induced by hurricanes and the prediction of so-called storm surges. This calculation was also done in 2010 by the ICES Computational Hydraulics Group led by Clint Dawson. The figure shows wind vectors and storm surge contours during Hurricane Katrina in 2005 that caused extensive flooding in southern Louisiana (Fig 19). The topography and bathymetry is generated using satellite images of the coast and sea-floor topography. On the right in Fig 21, we show the hypothetical transport of an oil spill if it had occurred during the storm. The coastal flooding is simulated by a finite element code called ADCIRC on a mesh of around ten million finite elements. The oil spill transport is represented by ten million Lagrangian particles. Coastal flooding is simulated with a one-second time-step over a span of seven days. It is solved using a fourth-order Runge-Kutta scheme and interpolating the computer currents over the same span. Had an oil spill been active during the landfall of Hurricane Katrina, oil would have been pushed further offshore and very near metropolitan New Orleans. With such calculations, we hope to quantify the hazards associated with coastal flooding during extreme, natural, and manmade events.

■ Nano-Manufacturing – Engineering at the Atomic Scale

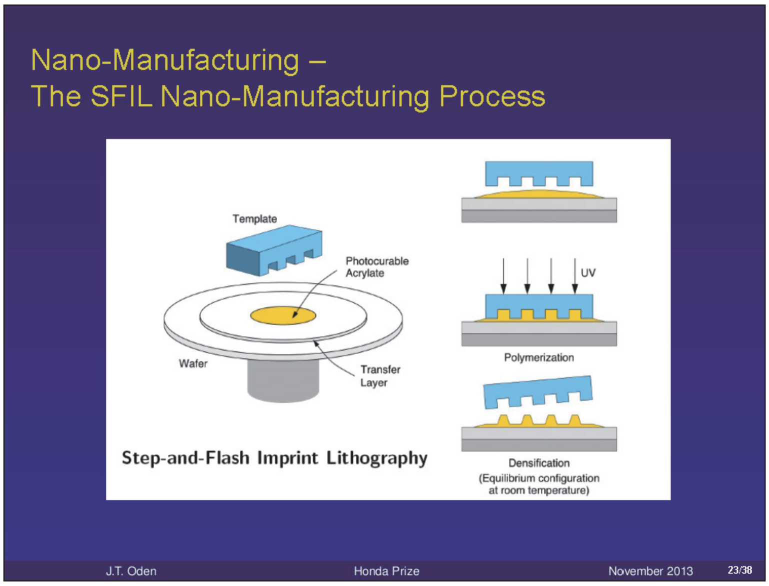

Fig 22

■ Nano-Manufacturing – Etch Barriers in Step and Flash Imprint Lithography

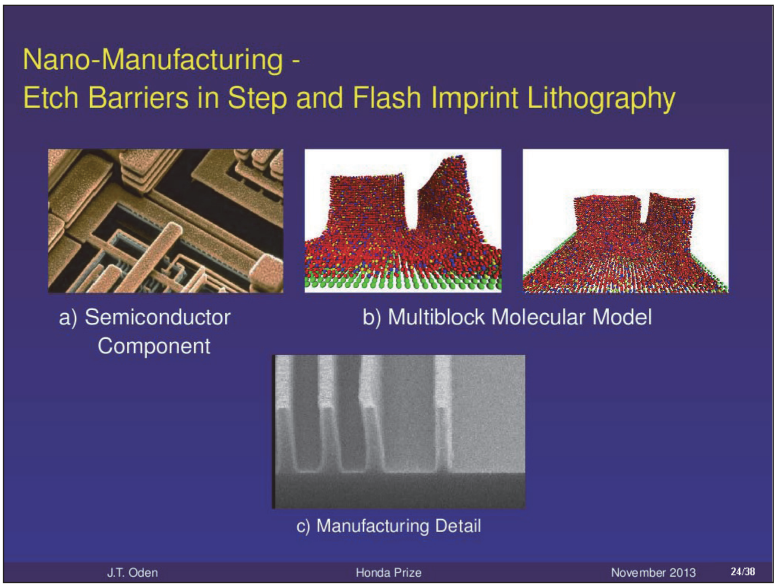

Fig 23

〈Fig 22-23〉 Computer modeling and simulation allows one to predict events and design engineering systems at scales perceptible only by electron microscopy. These types of models have been developed by my Multi-Scale Modeling Group at ICES and are used to simulate manufacturing objects at nanometer scales, ranging from nanoparticles for drug delivery to manufacturing today's semiconductor devices. It is known that the optimal speed of contemporary super computers depends upon the number of semiconductors that can be placed on a computer chip. So the grand challenge of modern chip design is to develop processes to produce smaller and smaller semiconductors – but this can only be done with careful designs and process monitoring of the manufacturing process.

Shown in the figure 22 is an example of a nanomanufactuing process at the nanoscale (which concerns subjects sized at one billionth of a meter, or 1000th the width of a human hair). The process, called Step and Flash Imprint Lithography, works by depositing a photocurable acrylate solution on a wafer that is exposed to ultra-violet light through a quartz template designed to imprint geometric features of tiny semiconductor components. The template and device involved in the process run upwards of $20 million and must be designed with precision to produce components of nanodimensions with almost perfect geometric fidelity.

The process of producing the critical etch barriers, shown, is modeled using a huge computational model of the polymer material (Fig 23). The model is used to define the shape of key semiconductor components.

■ Nano-Manufacturing – One Realization of the Polymerization Process

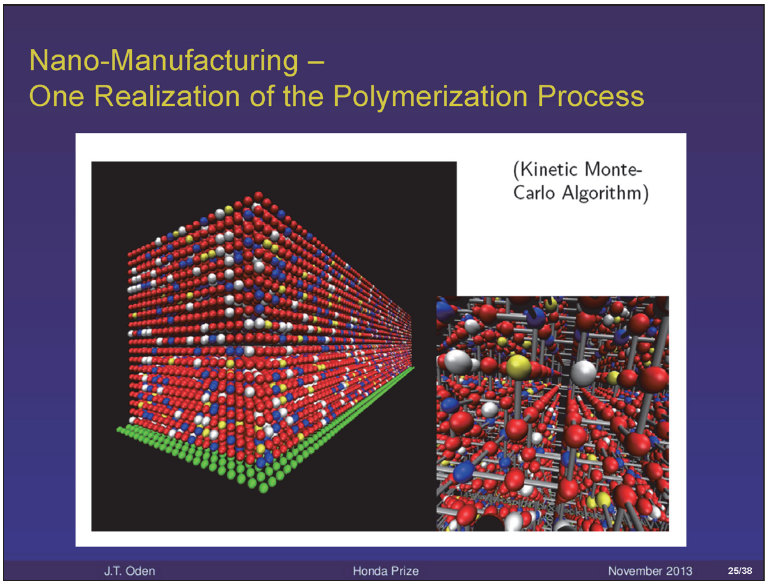

Fig 24

■ Nano-Manufacturing – Multi-Processor Computations

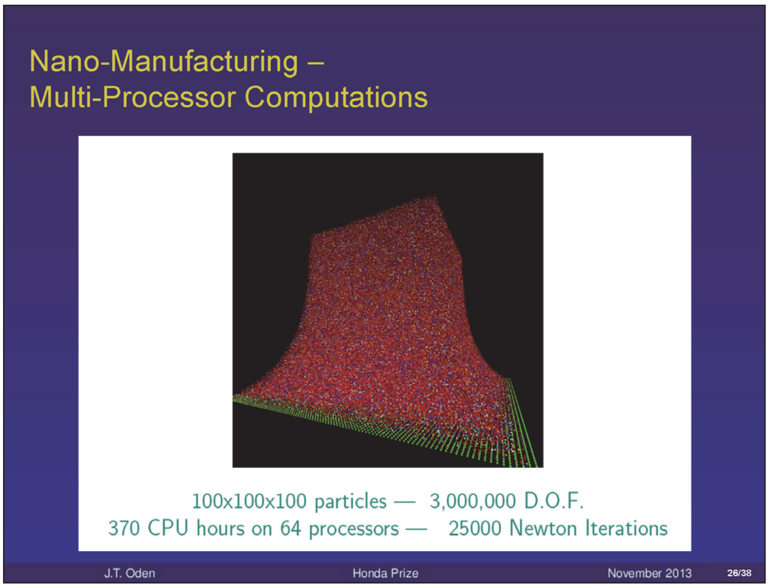

Fig 25

■ Nano-Manufacturing – Shrinkage Adaptive Step

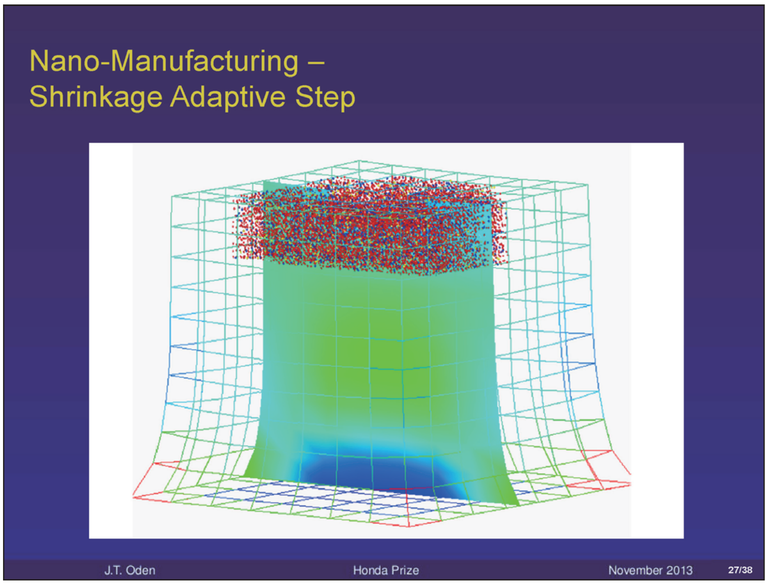

Fig 26

〈Fig 24-26〉 Computer generated molecular structures of the etch barrier are shown, attained using a Monte Carlo algorithm that employs kinetic chemical reaction rates to determine the most probable molecular situations (Fig 24). These structures are then introduced into a molecular dynamics model to compute the deformed shapes of the polymer barriers, as in the three-million-degree-of-freedom model shown (Fig 25).

A remarkable aspect of this calculation is that multi-scale modeling was used to control modeling error, resulting in hybrid models of the type shown where part of the structure was modeled at a molecular level and part at a macro-scale-continuous level (Fig 26). The resulting predictions helped optimize the design of the process and minimize flaws in the semiconductor components. This is an example of adaptive modeling that we developed to control error in predictions of component behavior.

■ Cardiovascular Modeling – Reconstruction of a 3D Anatomically Accurate Heart Mitral Valve

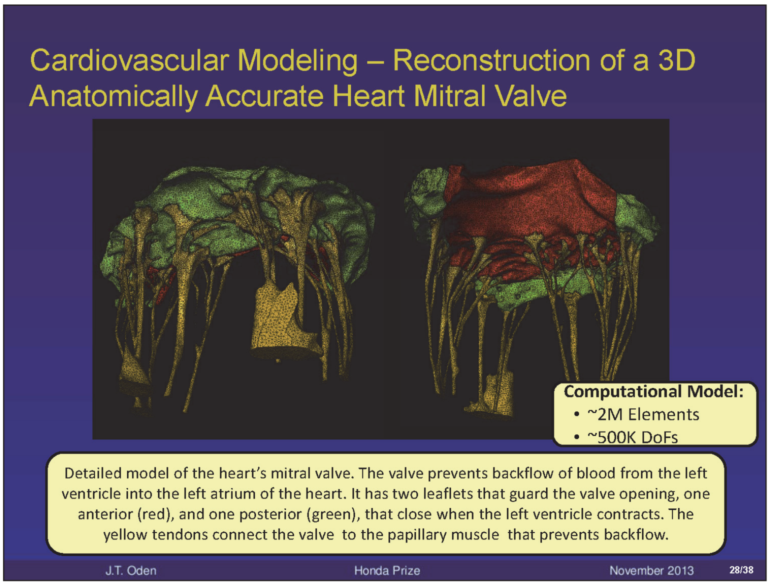

Fig 27

〈Fig 27〉 Next is a very interesting simulation of cardiovascular phenomena developed at the ICES Cardiovascular Simulation Center under the direction of Michael Sacks. This computational model is a reconstruction of an anatomically-accurate heart mitral valve. It was developed from a Micro CT image of around 39.46 microns resolution, with the perfect voxel resolution in around 1,014 slices. It shows the interior leaflet in red, the posterior leaflet in green, the chordae tendineaes and papillary muscles in yellow of the heart valve, with half a million nodes and around two million tetrahedral elements. The simplified model depicts the motion of the mitral valve this time using around 6,500 shell elements plus hexahedral elements for the mitral valve chordae tendineaes. The calculation was solved on 24 cores.

■ Cardiovascular Modeling – Mitral Valve Simulation

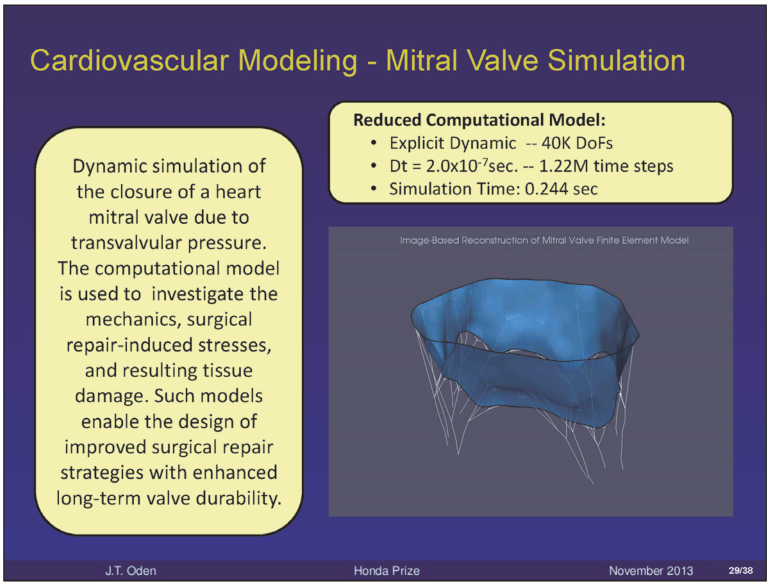

Fig 28

〈Fig 28〉 Here we see modeling and closure of the mitral valve due to trans-valvuler pressure–loading and ending with the thorough validation of the computational model using in vitro experimental data.

■ Prostate Cancer Research – A DDDAS Model – Cyberinfrastructure and Work Flow

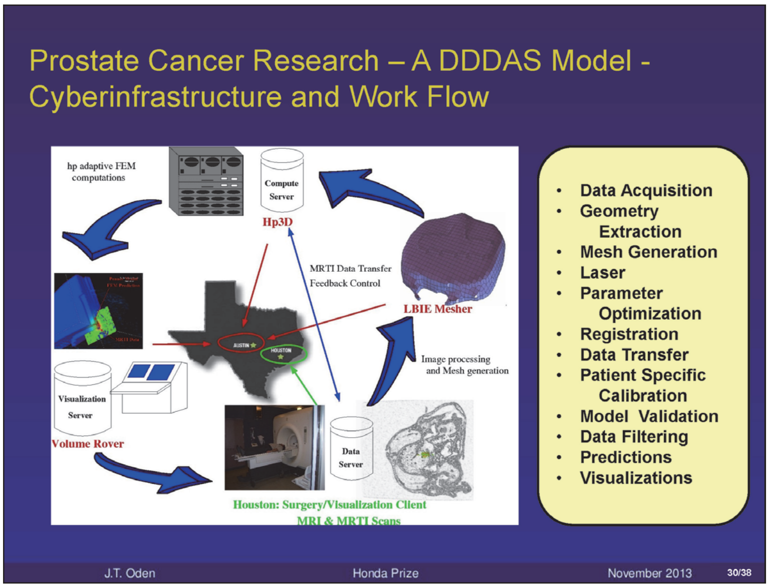

Fig 29

■ Prostate Cancer Research – A DDDAS Model – Imaging to Mesh Generation Pipeline

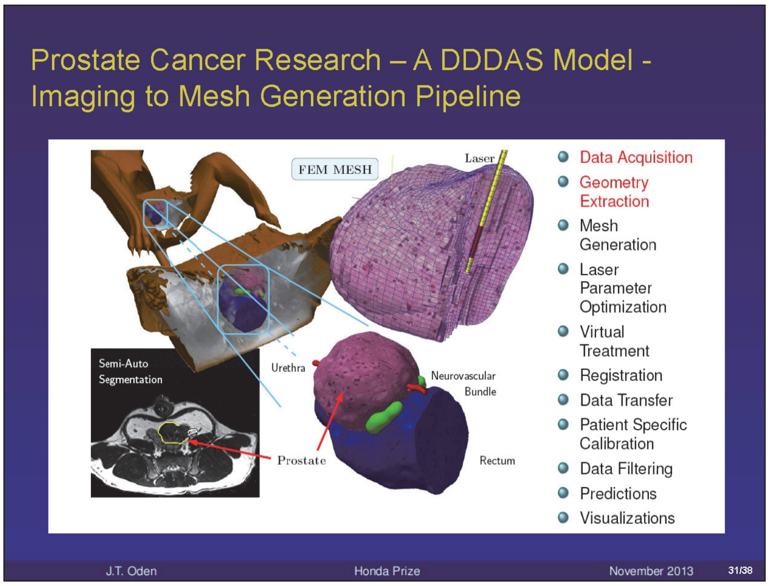

Fig 30

■ Prostate Cancer Research – A DDDAS Model – Patient Specific Calibration

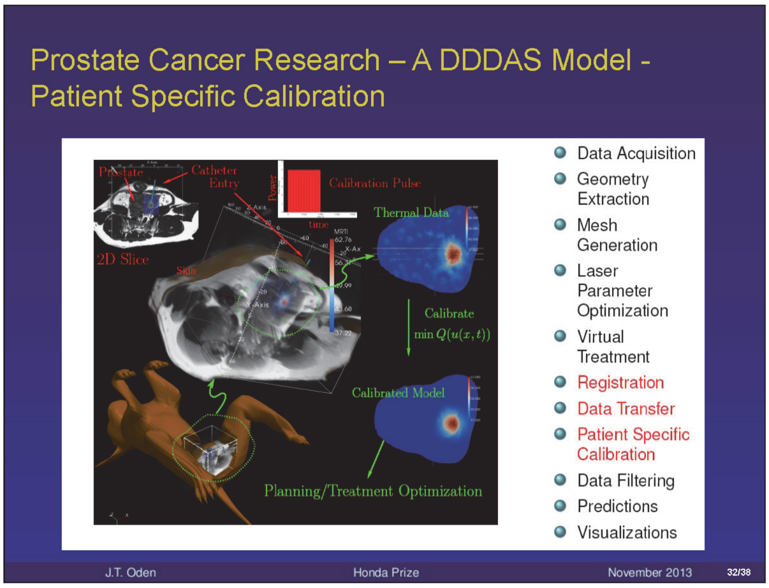

Fig 31

■ Prostate Cancer Research – A DDDAS Model –Treatment Process

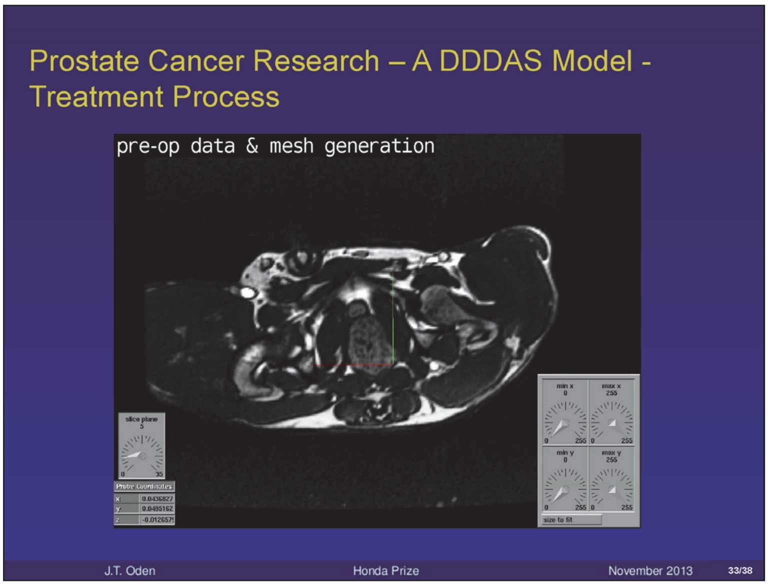

Fig 32

〈Fig 29-32〉 Here we see a dynamic data-driven application system designed to treat prostate cancer (Fig 29). The canine patient was placed in an MRI-device and an MRI image was taken of the infected prostate to be sent, over a high-bandwidth network, to the computational arena at ICES where a bioheat transfer model of the 3-D infected gland is made using finite elements and a model of bioheat transfer (Fig 30). The finite element mesh of the prostate shows a catheter inserted to terminate in the vicinity of the cancer cells. A laser was used to increase temperature in this area. Computational models of cell damage, heat shock protein, and thermal ablation were employed (Fig 31). By modeling the entire physical event, it is possible to minimize damage to healthy cells and maximize cancer cells in the vicinity of the catheter. The computational model enabled an adaptive control of the power of the laser, the resulting temperatures, the thermal environment supplied to the catheter, and the placement of the catheter in real time during this process. Next, very good agreement was obtained between the computational model and the experimental data, validating the models used. This study was conducted by my Multi-Scale Modeling Group at ICES.

■ Drug Design – SIV/HIV Envelope Interacting with a Candidate Inhibitor

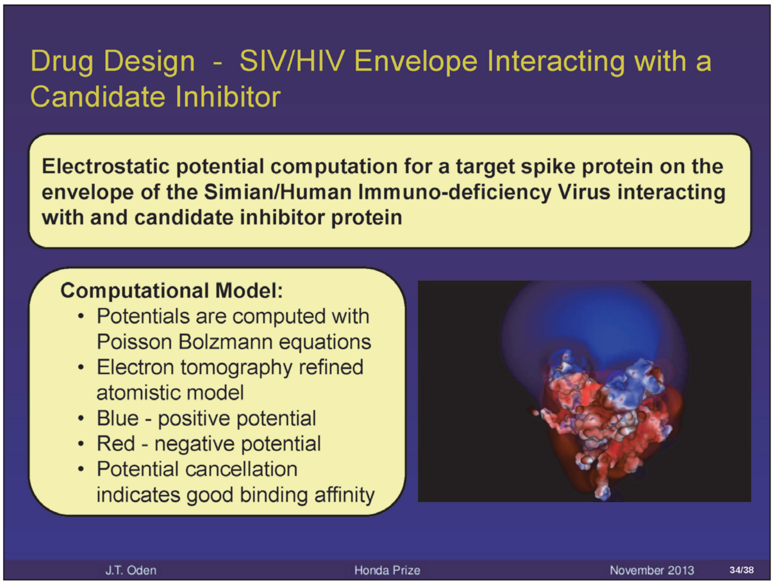

Fig 33

〈Fig 33〉 In the next example, we show results obtained by Chandrajit Bajaj's group in the Computational Visualization Center at ICES on electrostatic potential computations for a target-spiked protein GP120 on the envelope of SIV HIV simian immunodeficiency viruses interacting with a candidate inhibitory protein NIH45-46. HIV uses GP120 as an important signaling mechanism to gain simian-human immune T-cell entry. In the movie, the electrostatic potentials are computed with the Poisson-Boltzman equations initially using electron tomography for fine atomistic structure modeling of the GP120. Blue denotes positive potentials, red denotes negative potentials, and the cancelation of positive and negative potentials helps visualize the electrostatics complimentarity of the target and inhibitor and get the binding affinity.

■ HIV RT Synthesizes DNA

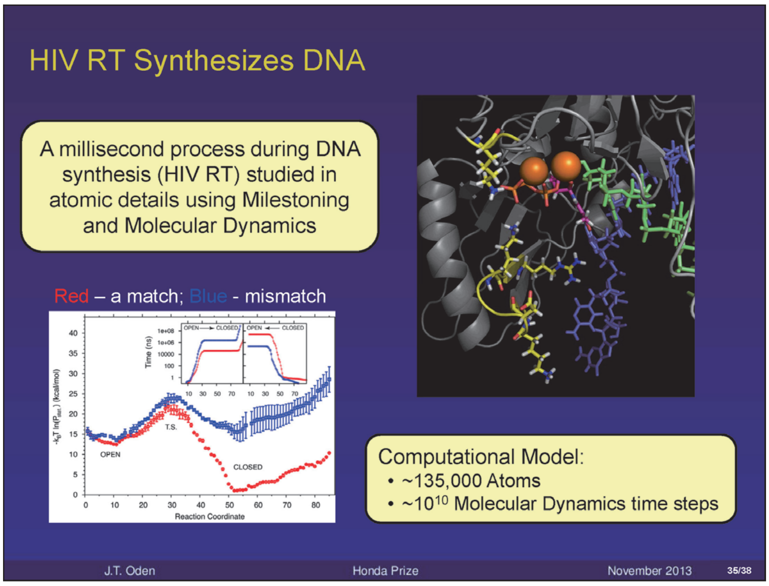

Fig 34

〈Fig 34〉 As a final example, we use computational methods to explore the secrets of life. Here, we display a minimum free-energy pathway for the conformational transition of the HIV reverse transcriptase obtained at ICES's Center for Computational Life Sciences and Biology directed by Ron Elber. HIV RT is a DNA polymerase with the task of synthesizing a new DNA molecule according to a template. The conformal transition of the protein when closing of a nucleotide is displayed. The transition selects the correct nucleotide to be added to the DNA. It is not completed successfully for the wrong substrate. Here, we were able to pinpoint the selection and reproduction quantitatively for the rate at which the protein changes its conformation to within milliseconds. The size of the model is 135,000 atoms. To compute the free-energy profile required around 10 billion molecular-dynamic steps with 10 femto-seconds for each time step. It was solved on the Lonestar computer at the Texas Advanced Computing Center running on 100 cores for over a month. What we see in the movie, is a close up of the protein active site and the way the protein changes its conformation while closing on the substrate. The group in purple is the nucleotide substrate to be added to the DNA in green. The orange spheres are magnesium ions necessary for the reaction, the yellow moving groups are positively-charged life sign side chains closing on a negatively charged nucleotide and getting it ready for chemical processing. What we hope to learn is how the protein selects the correct nucleotide to obtain an accurate copy of the original DNA. A conformational transition locks only on the correct substrate and the simulation makes it possible to quantify the locking mechanism that determines the rate of reaction in binding energy and the contribution to the overall precision of the enzyme. Some believe that this model can teach us the secrets of life with regard to the behavior of DNA and transport mechanisms. Membranes separate inside and outside cells, but nevertheless transportation across membranes is necessary to supply nutrients and eliminate waste products. One transport mechanism is passive, directly through the membrane, without the assistance of trans membrane proteins. Passive transport is also relevant for drug delivery. Here we consider the transport of a single amino acid tryptophan across a DOPC membrane as a model for permeants of moderate size.

■ Acknowledgements

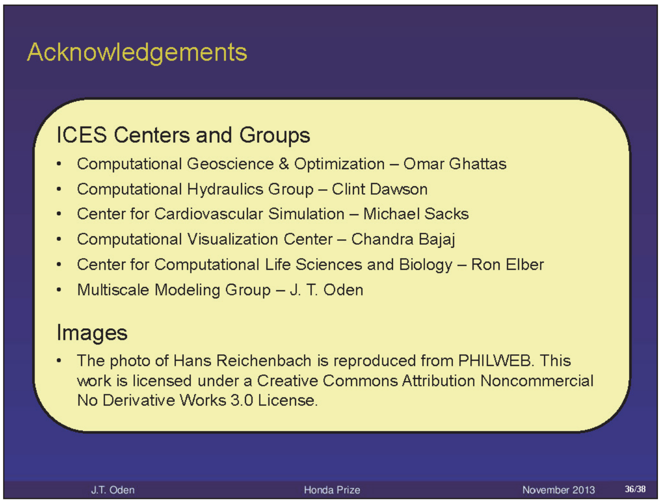

Fig 35

〈Fig 35〉 The examples I presented were kindly provided by my collaborators and colleagues and my group at ICES.

■ Summary and Conclusions

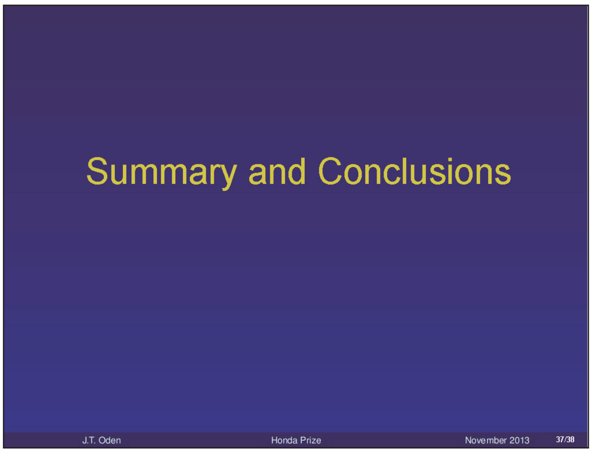

Fig 36

〈Fig 36〉 We are gradually coming to the realization that this Third Pillar will inevitably change the way we educate the scientists and engineers of the future, how we organize and perform research, and how we view knowledge and acquire it. The traditional compartments of knowledge reflected in our universities and in many industries is now seen to be artificial, not designed for interdisciplinary activities that are now made relevant and possible by the rise of computational science. The old systems will change or be lost in perpetuity.

What you and your children and your grandchildren will learn is that computational science will enable the study and understanding of things that have eluded scientists and engineers from the beginning. Can you study, with precision, events that happened centuries in past? Can you understand the initial and mechanical conditions that lead to earthquakes and tsunamis? Can you understand the stochastic nature of physical systems and have long-range predictions of our climate and our weather? Can you understand the nature of subatomic particles, of electrons, and how they form new materials? What about biological systems, such as the design and manipulation of new drugs, understanding diseases, the delivery of drugs at scales that cannot be perceived with the human senses? Can you model and understand the functions of the human body, the cardiovascular system, cures for cancer, or how to collect, store, process, and use the enormous amounts of data required to map out the functions of individual human bodies? Computational science has enabled all of these things to be lifted from the level of dreams and fiction and they are destined to become true accomplishments of science and technology in the future.

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