Perspectives on Materials Computational Science

Douglass Post

Los Alamos National Laboratory

International Workshop on Advanced Computational Materials Science for Nuclear Materials

Washington, DC

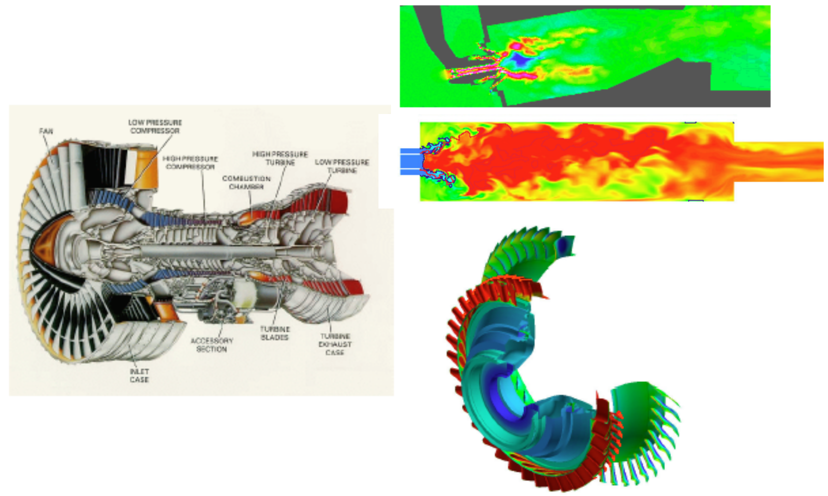
April 1, 2004

Revision of
LA-UR-04-0388

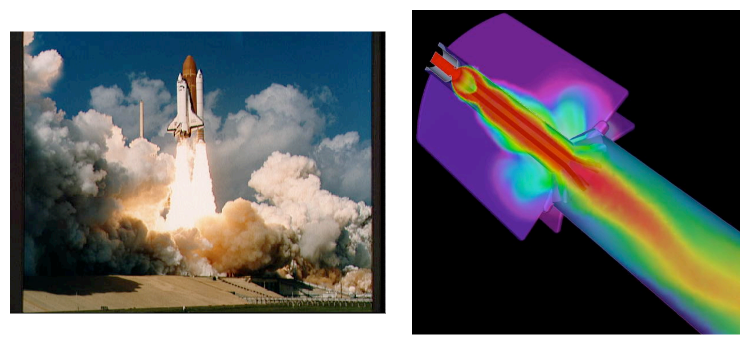
Approved for public release;
Distribution is unlimited

Introduction

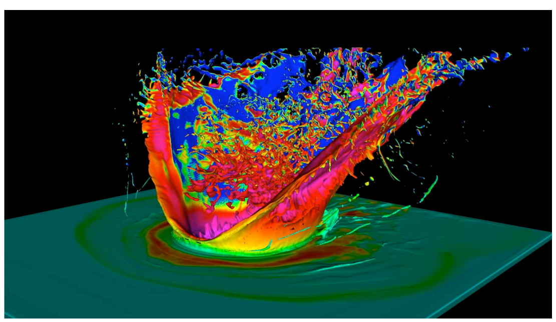
- Glad to be working with this community again. 25 years ago I was using sputtering data from TRIM and Marlowe to model tokamak divertors
- Computational materials have many of the same issues as the general computational science community
- The growth of computing power over the last 50 years has enabled us to address and “solve many important technical problems for society
- Codes contain Realistic models, good spatial and temporal resolution, realistic geometries, realistic physical data, etc. but we need to more than generate pretty pictures!



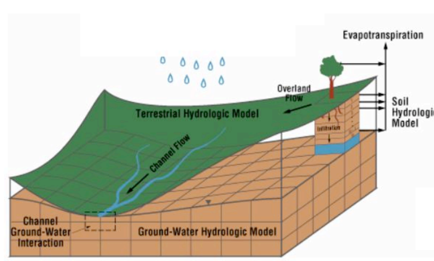
Stanford ASCI Alliance—Jet Engine Simulation



U. Of Illinois ASCI Alliance—Shuttle Rocket Booster Simulation

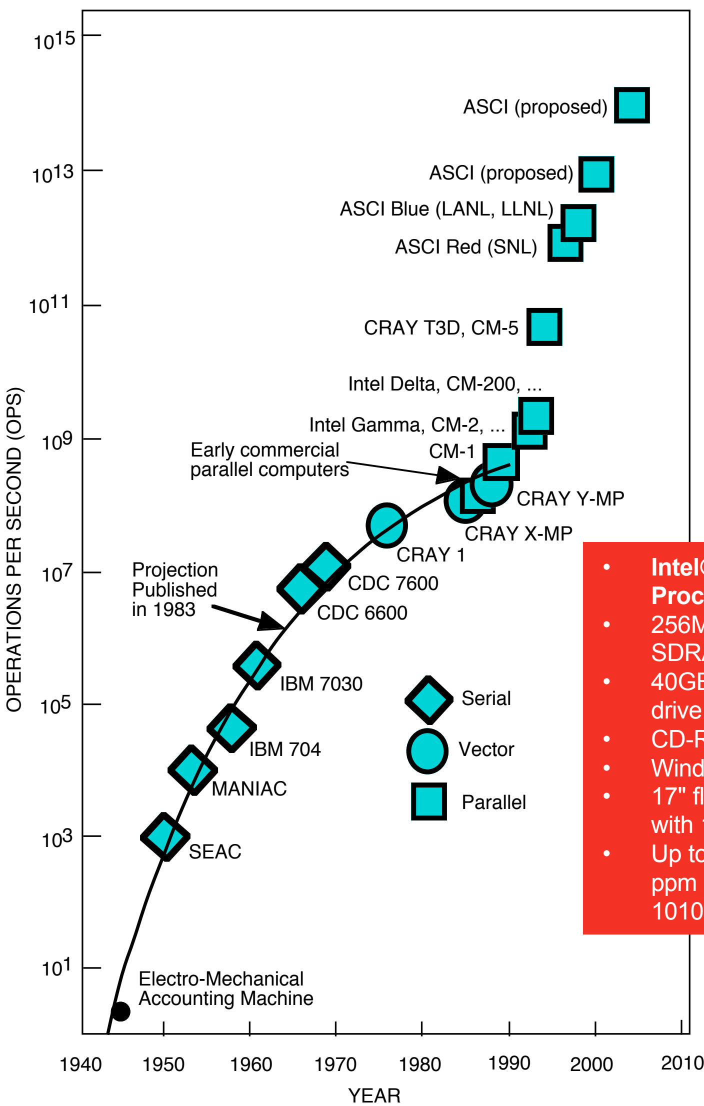


G. Gisler et al-Impact of Dinosaur Killer Asteroid



L. Winter et al-Rio Grande Watershed

Computer Power has increased 10^{13} since 1945



March 30, 2004

- **Intel® Celeron® Processor 2.7GHz**
- 256MB PC2100 DDR SDRAM memory
- 40GB Ultra DMA hard drive
- CD-RW drive—48x24x48x
- Windows® XP Home
- 17" flat screen monitor with 16" viewable area
- Up to 17 ppm black/12 ppm color printing Model 1010NX

Lessons Learned are important

- 4 stages of design maturity
- Case studies of failures (and successes) were essential for reaching reliability and credibility

Tacoma Narrows Bridge buckled and fell 4 months after construction!

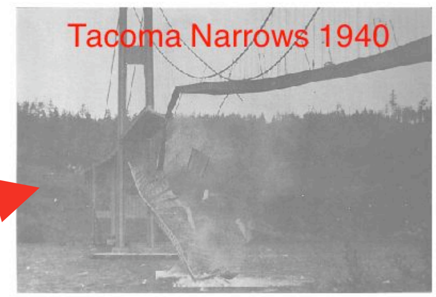
Case studies conducted after each crash.
Lessons learned identified and adopted by community

time

1

2

3



**Lessons Learned
Case Studies**

4

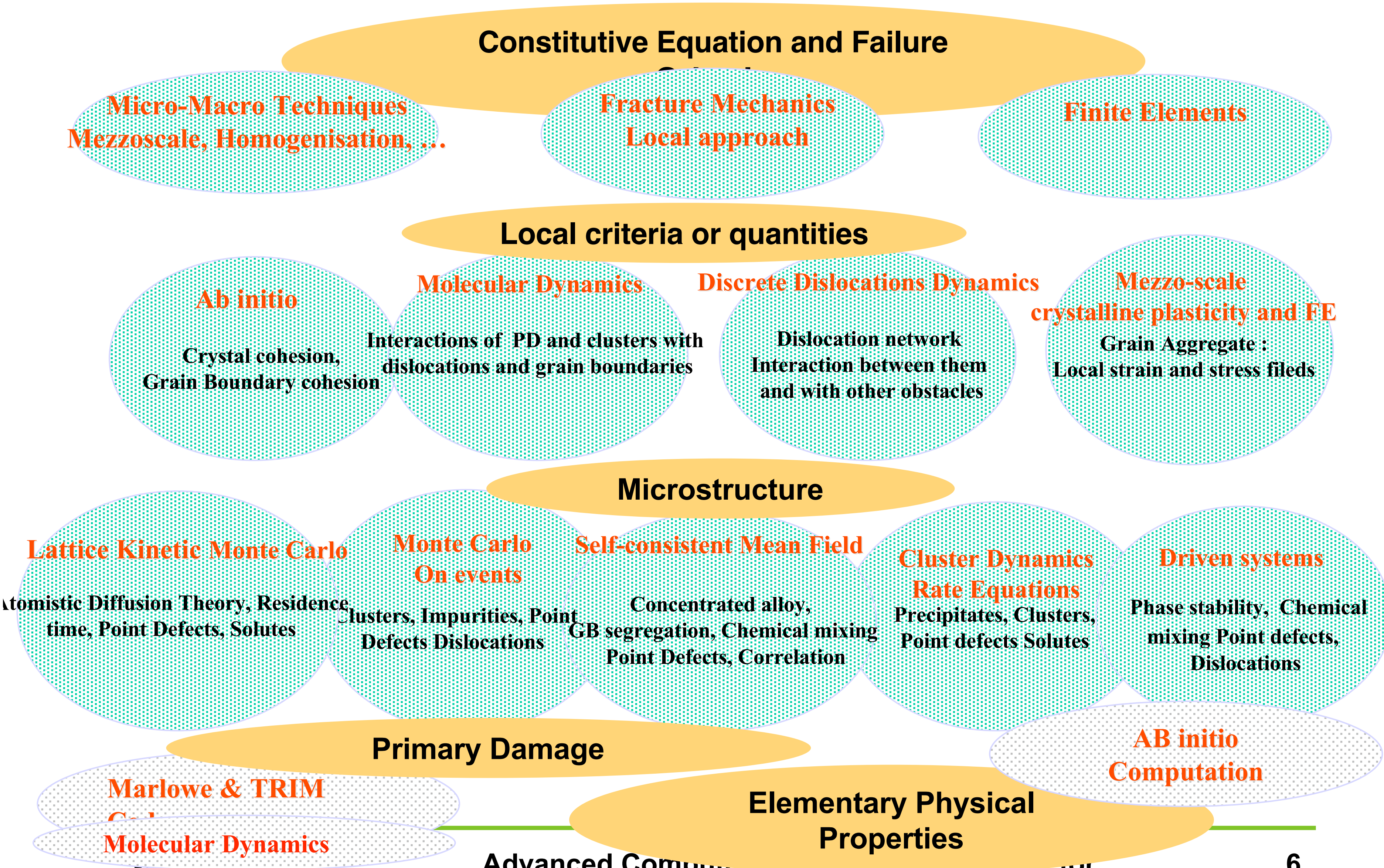
Case Studies: *"Lessons Learned"*

The Successful projects emphasized:

- Building on successful code development history and prototypes
- Highly competent and motivated people in a good team
- Risk identification, management and mitigation
- **Software Project Management: Run the code project like a project**
- Determine the Schedule and resources from the requirements
- Customer focus
  - For code teams and for stakeholder support
- Better physics and computational mathematics is much more important than better "computer science"
- The use of modern but proven Computer Science techniques,
  - They don't make the code project a Computer Science research project
- Develop the team
- **Software Quality Engineering: Best Practices rather than Processes**
- **Validation and Verification**

The unsuccessful projects didn't emphasize these.

Integration Sub-project: a unique architecture to compare performance & couple tools



—J.L. Boutard CEA/Saclay

Materials Simulation is entering new territory: a “Brave New World”

- **The past:**
  - **Small collocated teams**
  - **A limited number of effects in general**
  - **No deadlines or milestones**
  - **Peer review by community, etc.**
- **The future:**
  - **Big teams spread across many institutions,**
  - **Integrating many different effects,**
  - **Large projects that will likely have**
  - **Deadlines, milestones,**
  - **Oversight by regulatory bodies, etc.**

Welcome to the world of 10 CFR 830

- Software Quality Assurance mandated for codes used for nuclear safety and nuclear facilities.

issued August 5, 1998, are adopted as a final rule with the following change:

PART 1446—PEANUTS

1. The authority citation for part 7 CFR part 1446 continues to read as follows:

Authority: 7 U.S.C. 7271; 15 U.S.C. 714b and 714c.

2. Paragraph (c) of § 1446.102 is amended by adding a new sentence to the end of the paragraph to read as follows:

§ 1446.102 Administration.

* * * * *

(c) *Supervisory authority.* * * * Further, the Director of TPD, FSA, may authorize the wavier or modification of deadlines and other requirements, except statutory deadlines or requirements, in cases where lateness or the failure to meet such other requirements does not adversely affect operation of the program.

3. Paragraph (3) of the definition of "Segregations" in § 1446.103 is revised to read as follows:

§ 1446.103 Definitions.

* * * * *

(3) *Segregation 3.* Segregation 3 peanuts are farmers stock peanuts which, upon visible inspection, are found to contain Aspergillus flavus mold: *Provided further, however,* That, in accordance with such written instructions as the Director may issue, the Director shall permit producers at approved buying points as specified by the Director to have the Segregation 3 lot reconditioned, one time only, and then reinspected visually. If the buying point where the peanuts were initially delivered does not have adequate cleaning facilities, CCC may approve an alternative buying point for cleaning and reinspection. The visual reinspection may not occur more than 72 hours from the initial inspection except as permitted by the Director and the second grade shall be considered the final grade for the farmers stock peanuts.

§ 1444.307 [Amended]

4. Section 1444.307 is amended by removing paragraph (g) from that section.

Signed at Washington, D.C., on January 3, 2001.

Keith Kelly,

Executive Vice President, Commodity Credit Corporation.

[FR Doc. 01–651 Filed 1–9–01; 8:45 am]

BILLING CODE 3410–05–P

DEPARTMENT OF ENERGY

10 CFR Part 830

RIN 1901–AA34

Nuclear Safety Management

AGENCY: Department of Energy

ACTION: Final rule.

SUMMARY: The Department of Energy (DOE) adopts, with minor changes, the interim final rule published on October 10, 2000, to amend the DOE Nuclear Safety Management regulations.

EFFECTIVE DATE: This final rule is effective on February 9, 2001.

FOR FURTHER INFORMATION CONTACT: Richard Black, Director, Office of Nuclear and Facility Safety Policy, 270CC, Department of Energy, 19901 Germantown Road, Germantown, MD 20874; telephone: 301–903–3465; e-mail: Richard.Black@eh.doe.gov

SUPPLEMENTARY INFORMATION:

I. Introduction and Summary

On October 10, 2000, the Department of Energy (DOE) published an interim final rule in the **Federal Register** (65 FR 60291) that amended DOE's nuclear safety regulations in 10 CFR Part 830 (Interim Final Rule). DOE provided a 30-day public comment period for the Interim Final Rule and subsequently received comments to the rule from over 30 parties. As a result of the comments that were received to that Interim Final Rule, DOE became aware of a number of minor errors in the published version of the rule and the preamble, as well as a number of minor changes to the rule that would clarify and simplify implementation of the amended rule. We are republishing the rule as a final rule with those changes. Finally, we are summarizing the issues raised in the comments to the Interim Final Rule and providing DOE's responses to the major issues. Many of the comments concerned rule implementation issues that will be addressed in the rule implementation guides.

II. Discussion of Changes to the Rule

The following changes to 10 CFR Part 830 are being made in response to comments to the Interim Final Rule.

A. Changes to § 830.2, Exclusions

We are amending paragraph 830.2(d) to exclude the mixed oxide fuel fabrication and irradiation facilities that the Nuclear Regulatory Commission (NRC) has the authority to license and regulate under § 3134 of the Strom Thurmond National Defense Authorization Act for Fiscal Year 1999 (Public Law 105–261). Section 3134 amends the Energy Reorganization Act of 1974 to add § 202(5) (42 U.S.C. 5842). This exclusion will make clear that these facilities will be licensed by the NRC and must be designed and constructed to meet NRC regulations. Thus, these facilities are excluded from the requirement to meet 10 CFR Part 830 before and after a license is issued by the NRC.

B. Changes to § 830.3, Definitions.

We are revising the following definitions in § 830.3:

1. Safety Class Structures, Systems, and Components

We are revising the words "identified by the documented safety analysis" to "determined from safety analyses" to make the definition consistent with those for "safety structures, systems, and components" and "safety significant structures, systems, and components."

2. Technical Safety Requirements (TSRs)

We are revising the definition of TSRs to express it more clearly. As revised, the definition of TSRs means the limits, controls, and related actions that establish the specific parameters and requisite actions for the safe operation of a nuclear facility and include, as appropriate for the work and the hazards identified in the documented safety analysis for the facility: Safety limits, operating limits, surveillance requirements, administrative and management controls, use and application provisions, and design features, as well as a bases appendix. The documented safety analysis identifies the need for TSRs, but the actual limits are identified in the TSRs. The revisions make clear that the TSRs address the specific numerical limits and related actions necessary for safe operation of a nuclear facility. Because the TSRs identify the limits and actions necessary in specific situations, it is not appropriate to use the graded approach to justify the use of different limits and actions than those set forth in the TSRs. The change made to the graded approach section is consistent with this change.

C. Changes to § 830.7, Graded Approach

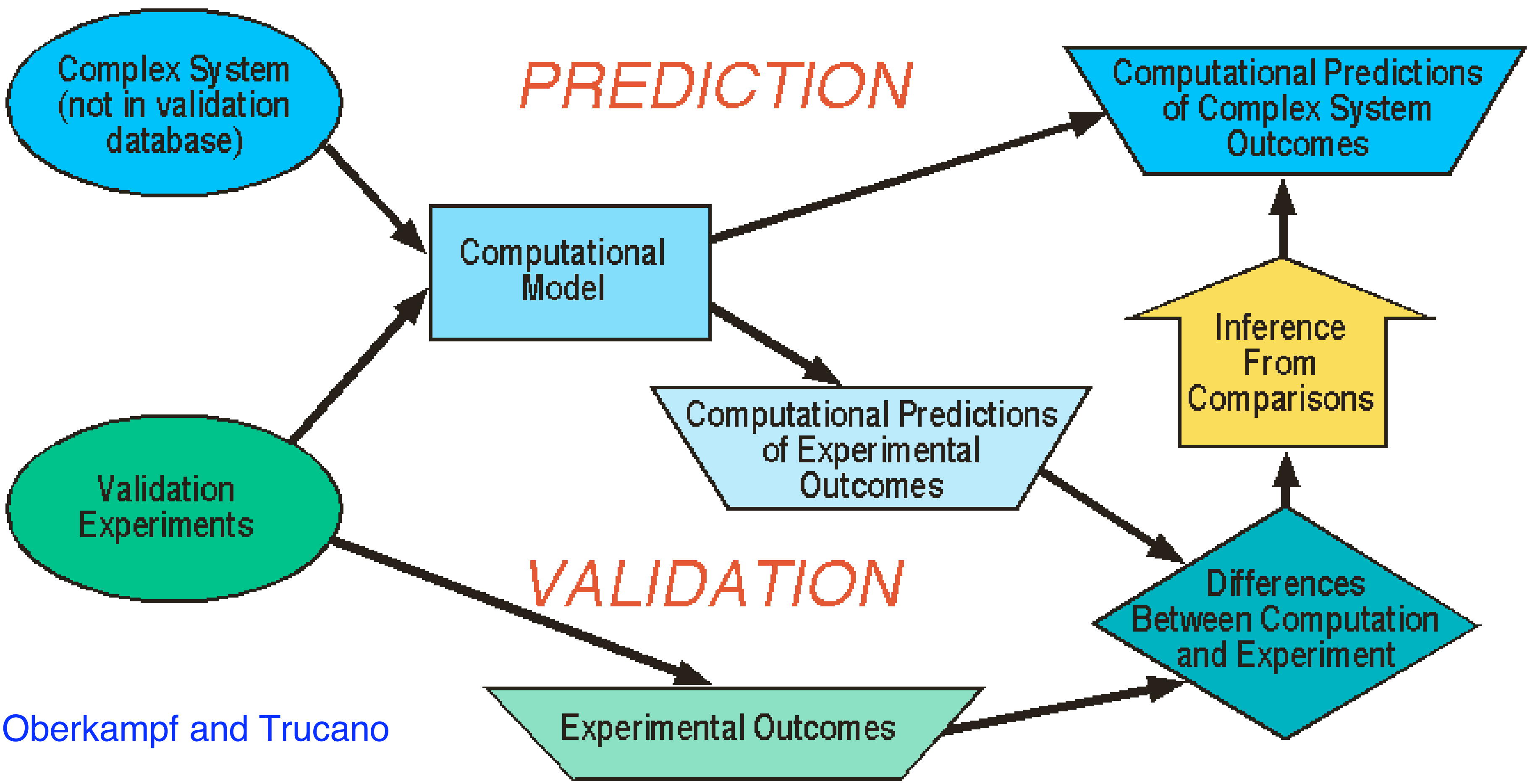
We received a number of comments requesting us to clarify where a contractor must use a graded approach and how the graded approach documentation should be submitted. We are revising the language in § 830.7 to clarify that a contractor may not use a graded approach in implementing the unreviewed safety question (USQ)

Verification is essential.

- Verification-the code solves its model correctly
- If it doesn’t do that, validation is a waste of time
- How?
  - Exercise care, review code, monitor code for unusual behavior
  - Check with analytic test problems
  - Convergence tests
  - Manufactured solutions
  - Monitor conserved and predictable processes
- There isn’t much else. What do you do?

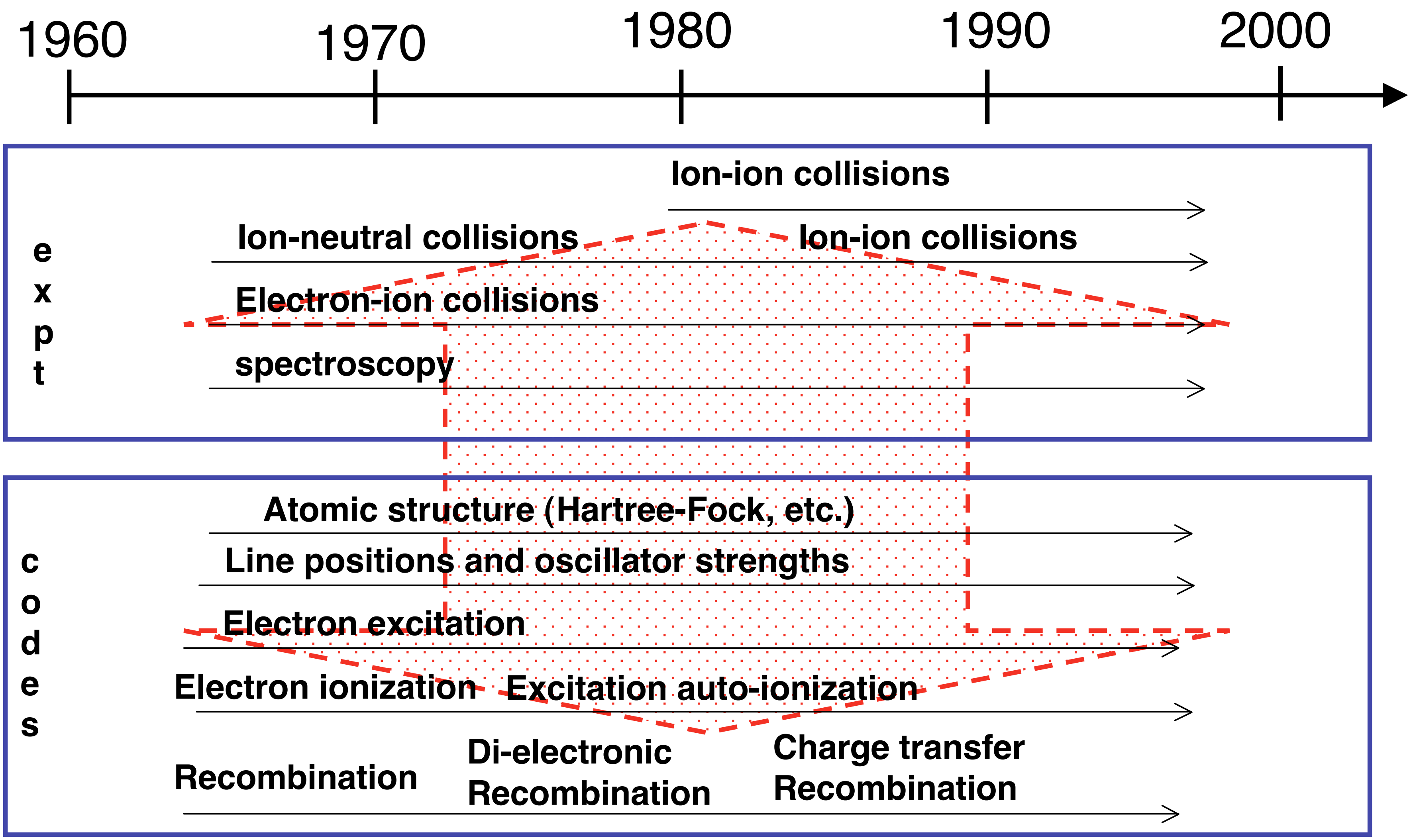
Predictive capability is linked to validation experiments.

- Predictions for validation experiments are essential



— Oberkampf and Trucano

International Atomic Physics Community (Astrophysics and fusion)

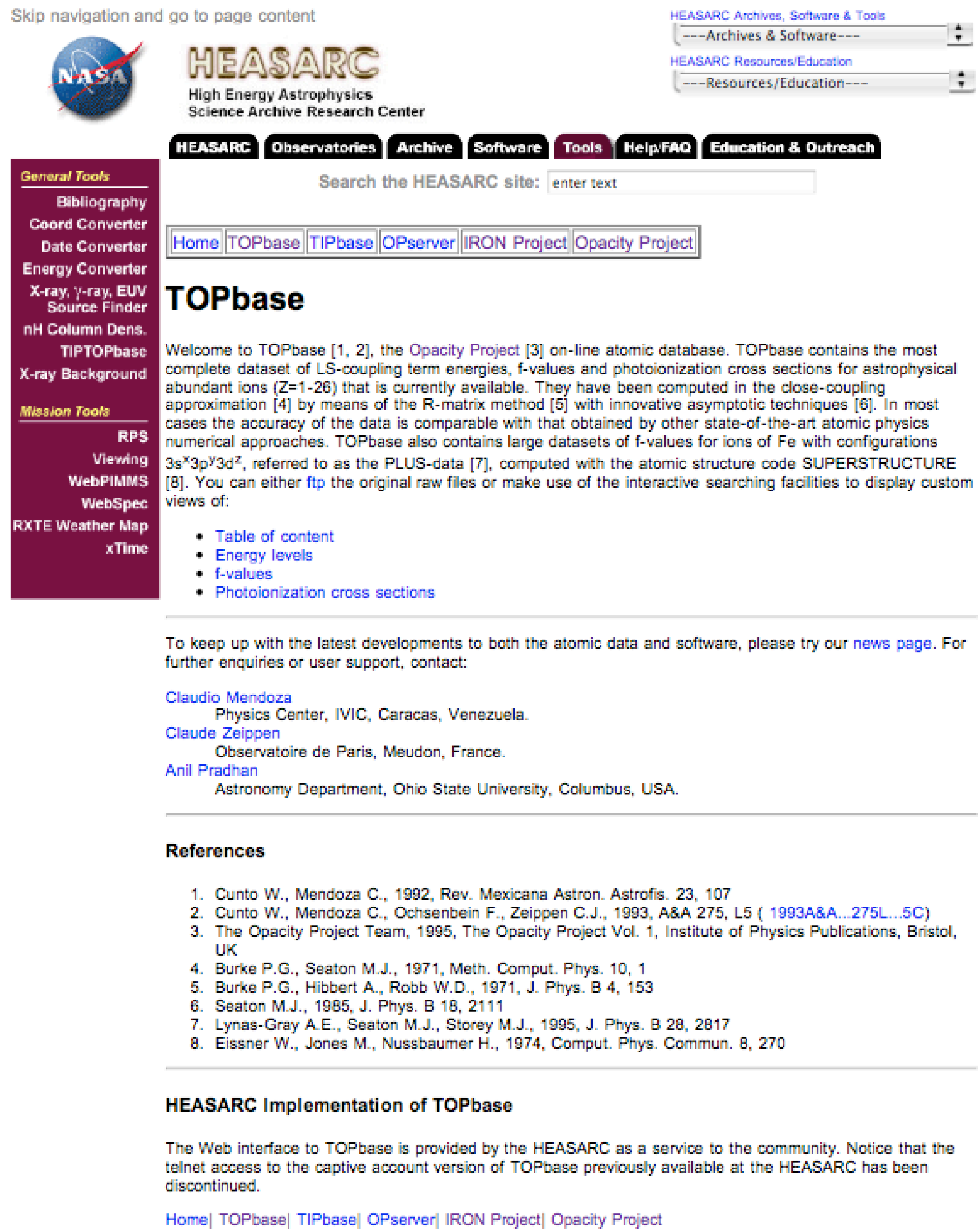


“Virtual” International Projects
Iron Project
Opacity Project

Many institutions
- UK: London, Belfast
- US: JILA, Harvard, NASA, NBS,….
- Japan, France, Germany, Many others

- Long term, began in 1960’s, going strong today
- Free sharing of codes, packages, modules
- Low level of formality
- Common interests and benefit, strong scientific reputation of leaders

- No real proprietary issues (not a large lucrative market)



Skip navigation and go to page content

HEASARC
High Energy Astrophysics
Science Archive Research Center

HEASARC Archives, Software & Tools
---Archives & Software---
HEASARC Resources/Education
---Resources/Education---

HEASARC | Observatories | Archive | Software | Tools | Help/FAQ | Education & Outreach

Search the HEASARC site: enter text

General Tools
Bibliography
Coord Converter
Date Converter
Energy Converter
X-ray, γ-ray, EUV Source Finder
nH Column Dens.
TIPTOPbase
X-ray Background

Mission Tools
RPS
Viewing
WebPIMMS
WebSpec
RXTE Weather Map
xTime

Home | TOPbase | TIPbase | OPserver | IRON Project | Opacity Project

TOPbase

Welcome to TOPbase [1, 2], the Opacity Project [3] on-line atomic database. TOPbase contains the most complete dataset of LS-coupling term energies, f-values and photoionization cross sections for astrophysical abundant ions (Z=1-26) that is currently available. They have been computed in the close-coupling approximation [4] by means of the R-matrix method [5] with innovative asymptotic techniques [6]. In most cases the accuracy of the data is comparable with that obtained by other state-of-the-art atomic physics numerical approaches. TOPbase also contains large datasets of f-values for ions of Fe with configurations $3s^x3p^y3d^z$, referred to as the PLUS-data [7], computed with the atomic structure code SUPERSTRUCTURE [8]. You can either ftp the original raw files or make use of the interactive searching facilities to display custom views of:

- Table of content
- Energy levels
- f-values
- Photoionization cross sections

To keep up with the latest developments to both the atomic data and software, please try our news page. For further enquiries or user support, contact:

Claudio Mendoza
Physics Center, IVIC, Caracas, Venezuela.
Claude Zeippen
Observatoire de Paris, Meudon, France.
Anil Pradhan
Astronomy Department, Ohio State University, Columbus, USA.

References

1. Cunto W., Mendoza C., 1992, Rev. Mexicana Astron. Astrofis. 23, 107
2. Cunto W., Mendoza C., Ochsenbein F., Zeippen C.J., 1993, A&A 275, L5 (1993A&A...275L...5C)
3. The Opacity Project Team, 1995, The Opacity Project Vol. 1, Institute of Physics Publications, Bristol, UK
4. Burke P.G., Seaton M.J., 1971, Meth. Comput. Phys. 10, 1
5. Burke P.G., Hibbert A., Robb W.D., 1971, J. Phys. B 4, 153
6. Seaton M.J., 1985, J. Phys. B 18, 2111
7. Lynas-Gray A.E., Seaton M.J., Storey M.J., 1995, J. Phys. B 28, 2817
8. Eissner W., Jones M., Nussbaumer H., 1974, Comput. Phys. Commun. 8, 270

HEASARC Implementation of TOPbase

The Web interface to TOPbase is provided by the HEASARC as a service to the community. Notice that the telnet access to the captive account version of TOPbase previously available at the HEASARC has been discontinued.

Home| TOPbase| TIPbase| OPserver| IRON Project| Opacity Project

Complementary role of experiments and simulation and theory

Astron. Astrophys. Suppl. Ser. **143**, 483{489 (2000)

Atomic data from the IRON Project

XLII. Electron impact excitation of Fe xxi

K. Butler[1] **and C.J. Zeippen**[2]

[1] Institut f¨ur Astronomie und Astrophysik, Scheinerstr. 1, D-81679 M¨unchen, Germany

[2] UMR 8631 (associ ee au CNRS et a l'Universit e Paris 7) et DAEC, Observatoire de Paris, F-92195 Meudon, France

- Example: spectroscopy
- Zillions of lines for 1000's of ions (Fe^{+q}, 0<q<26; W^{+q}, 0<q<74)
- Experiments establish the positions and line strengths of a small number of lines
- Simulations generate the full data set of lines and line strengths (see the NBS tables, etc.)

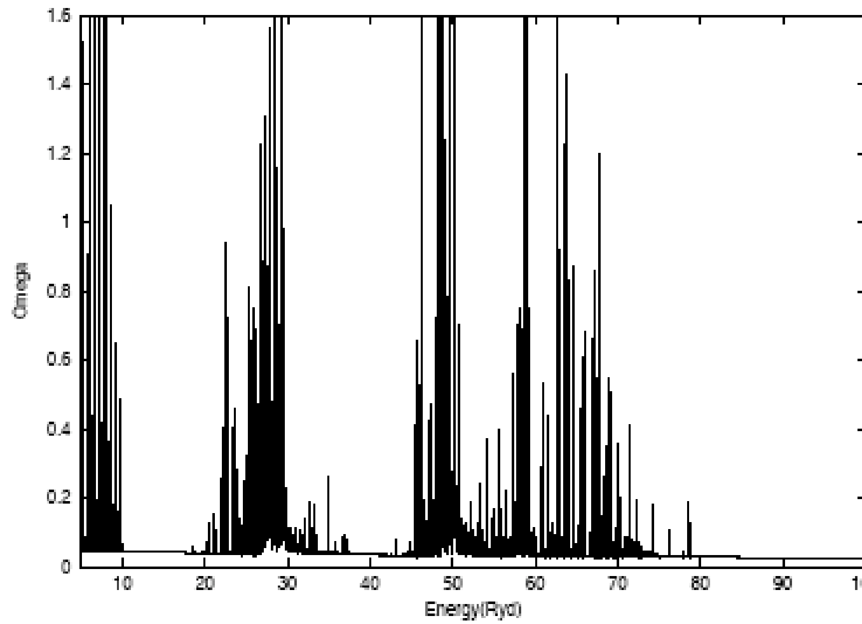


Fig. 4. The $2s^2 2p^2\ {}^3P^e_1 - {}^3P^e_2$ collision strength at high energies. These resonances do not appear in the Aggarwal (1991) calculation

Path Forward

- Appropriate role of simulation expressed in many talks here, Olson in particular
- Codes capture the corporate knowledge and understanding
- But code results must be sufficiently reliable that one can base decisions on their results
- Codes are only models of nature, not nature
  - Unvalidated codes are useless
- Codes complement experiments
- Experiments are expensive, time consuming, can't easily use experiments to map out parameter space, explore all possible options
- Codes can fill in gaps between experimental benchmarks, explore new parameters, confirm understanding and ability to extrapolate from existing knowledge
- Progress proceeds in a "leap frog" fashion, experiments working together with codes/theory, each feeding the other with results, understanding, models and hypotheses, to develop a predictive capability

Codes and experiments are both essential for progress

- In my view, validation will need dedicated experiments that can test the ability of the codes to predict
  - Validation will need to more to a more formal basis: projects with clearly defined goals and documented achievements
  - Ability to predict both single physics and integrated physics effects will need validation
- For fission and fusion: prototypical spectra and fluxes and material conditions (temperatures, etc.) to confirm understanding of relevant mechanisms and provide benchmarks to validate the codes
  - Fission: reactors are essential
  - Fusion: a 14 MeV neutron source is essential
- Codes can be used to optimize the experimental program and reduce the required experimental **capacity** but not the experimental **capability**
- The experiments will need the capability to benchmark and validate the codes, and provide confirmation that the choices made on the basis of code results were correct

Do we have the right algorithms?

- Many of the algorithms don't scale well for present 1000 to 10,000 processor machines.
- How are we going to make the shift to algorithms that work well on 100,000 processors?

Other computational communities emphasize validation

- DOE/NNSA spending much more on validation experiments than on modelling
  - National Ignition Facility (NIF), ~$3B capital cost, ~$350M/year operating costs
  - Dual Axis Radiograph, Z, Omega, Trident,….
- Main purpose of NIF is to validate nuclear weapons design codes

- CFD community using dedicated wind tunnels
- Many other communities using simulation for decisions
  - Engineering communities do design with codes
  - Each new type of application is validated, each element **and** the integrated package
- All require validation!
- We also need validation.