Supernovae: Elements of Theory, Computations, Experiments

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Outline

- Lecture 1
- Lecture 2
- Lecture 3

Outline

- Lecture 1: Experimental Astrophysics
- Lecture 2: Core-collapse Supernovae
- Lecture 3: Thermonuclear Supernovae

Outline

- Lecture 1: 70 minutes
- Lecture 2: 40 minutes
- Lecture 3: 40 minutes

Lecture 1

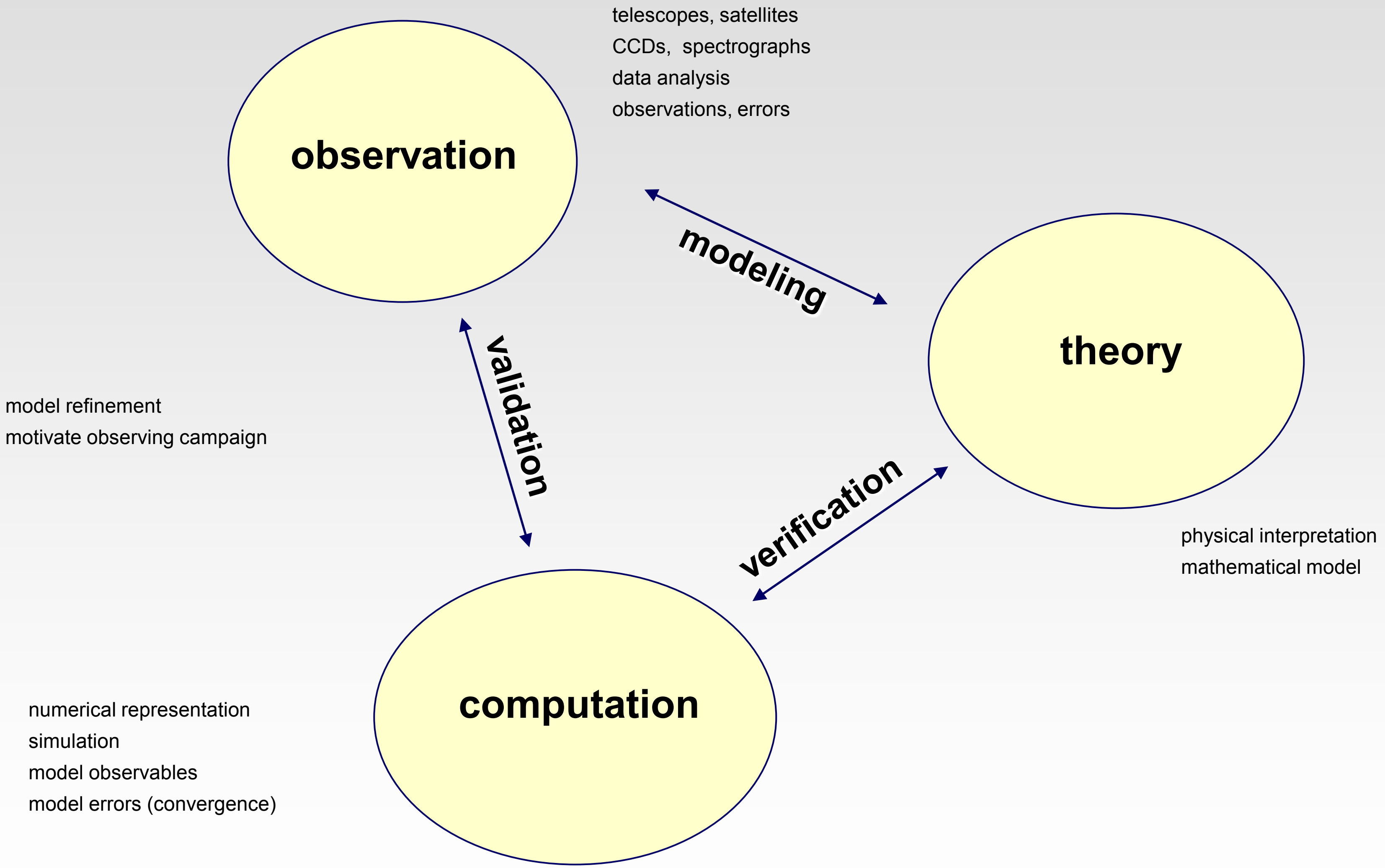
Verification & Validation:
Toward Reliable Computations

“So far, so good…”

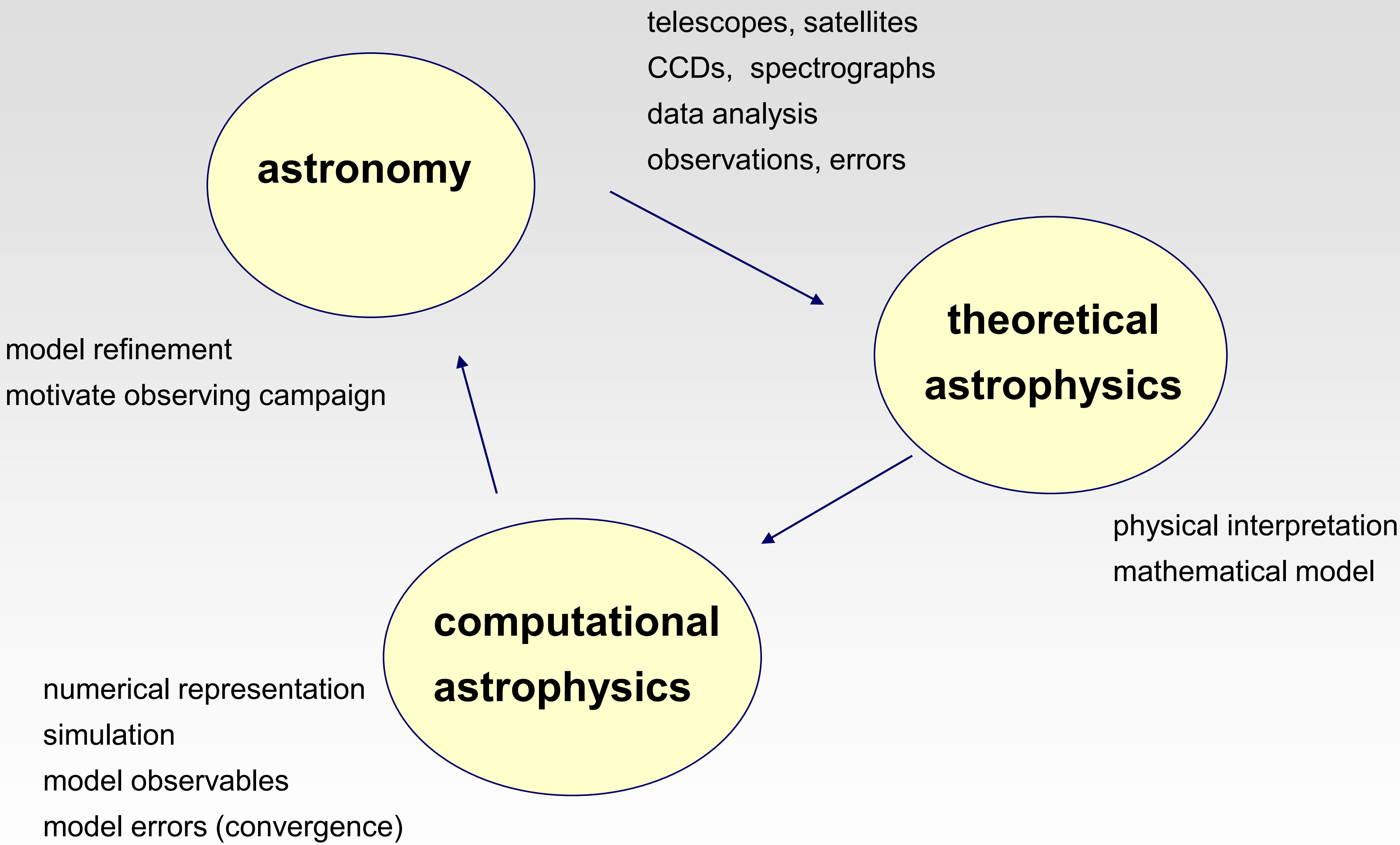
- Experiments: the first 3 talks
- Equilibrium “soup”, EOS: Rafelski’s talk
- PDE: Birell’s talk
- Limits and errors, sampling: Sikora’s talk

- …and it’s about to get even better!

Three Legs of Modern Science

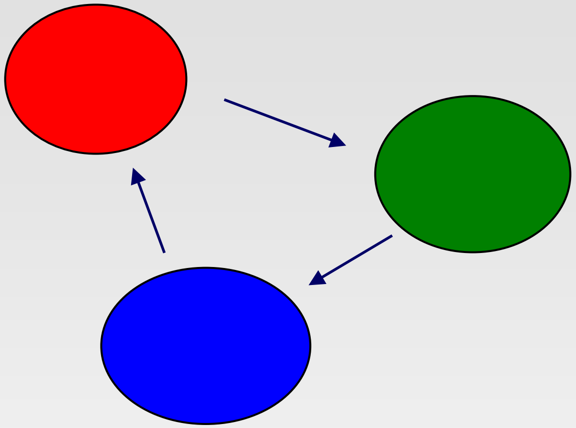


Astronomy & Astrophysics



Production Cycle Elements

- **Observation**
- **Modeling**
  - Conceptual model
  - Mathematical model
  - Algorithmic development
- **Software implementation**
  - Implementation verification
  - Solution verification
  - Code maintenance (test suite, cvs/svn)
- **Simulation**
  - Simulation results
  - Sensitivity Analysis
  - Uncertainty Quantification
  - Validation
  - Data analysis (visualization, analytics)



Astronomy: Explosive Observations

- Classical Novae
- Thermonuclear Supernovae (Type Ia)
- Core-collapse Supernovae (Type II & Ib/Ic)
- Gamma-ray bursts
- X-ray bursts

Astrophysics: Theory & Computations

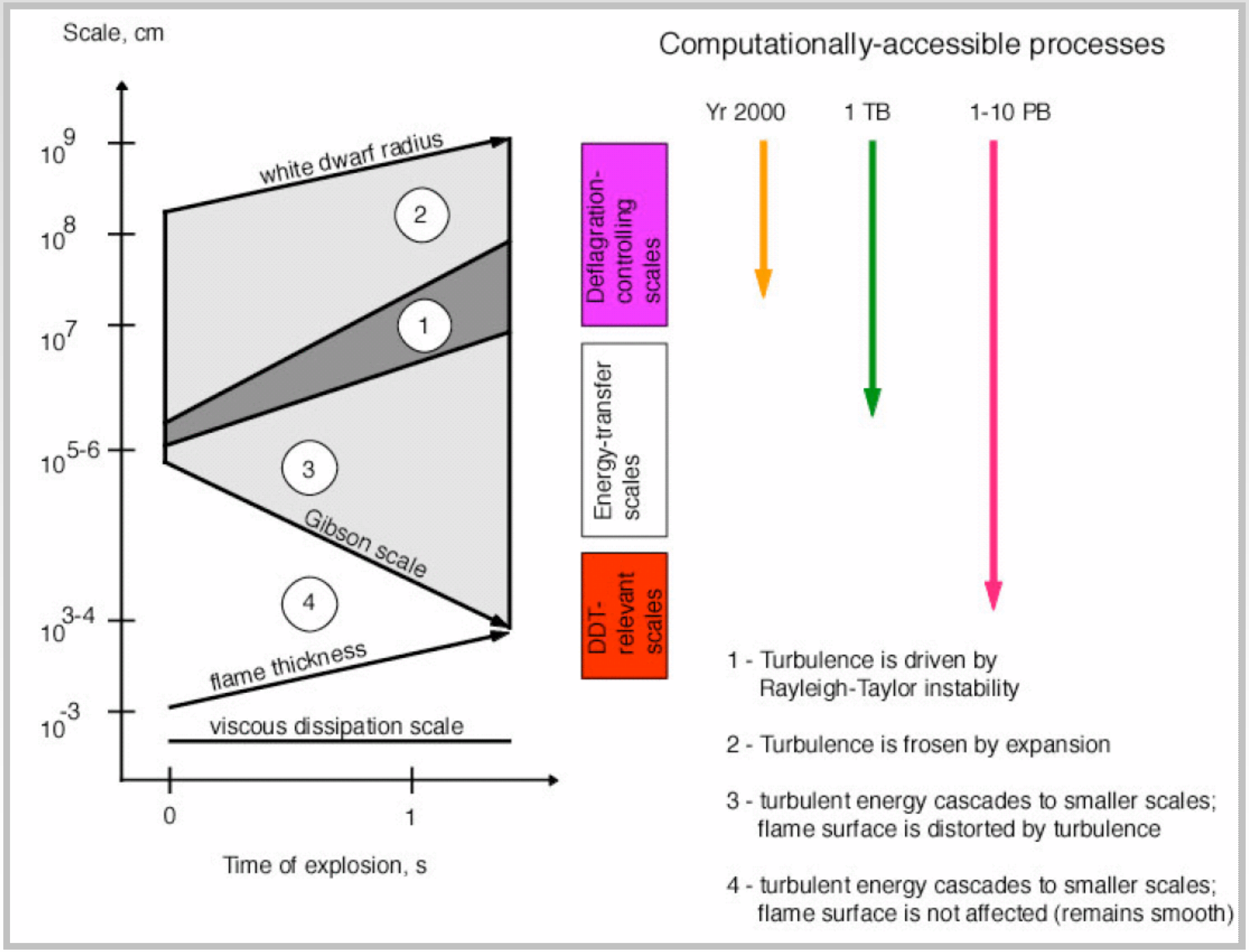
Theory

- Motivated by observation, stimulated by computations

- Pure, magneto-, radiation-, SR, and GR hydrodynamics
- Evolutionary processes of large stellar assemblies
- Plasma physics
- Radiative processes
- N-body gravitational systems
- Chemistry of interstellar matter, molecular clouds
- Nuclear physics
- Data (image, spectral) analysis

- Linearization
- Higher-order perturbative analysis
- Order of magnitude estimates
- Statistics

Orders of Magnitude (SN Ia)



Khokhlov (2003)

Computations

$$\partial_t \mathbf{U} + \nabla \mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U})$$

$$\nabla^2 \Phi = 4\pi G \rho$$

- **PDEs** of every possible type
- **ODEs** frequently stiff
- complex equation of state (first closure relation)
- **strongly coupled**
- **multidimensional** (4D...7D, more closure relations)
- various discretization methods (finite volume solvers, multigrid, particles, subgrid, front tracking)
- adaptive in space and time
- prone to produce demonstration runs
- unlimited computing resources ("**tree barking**")

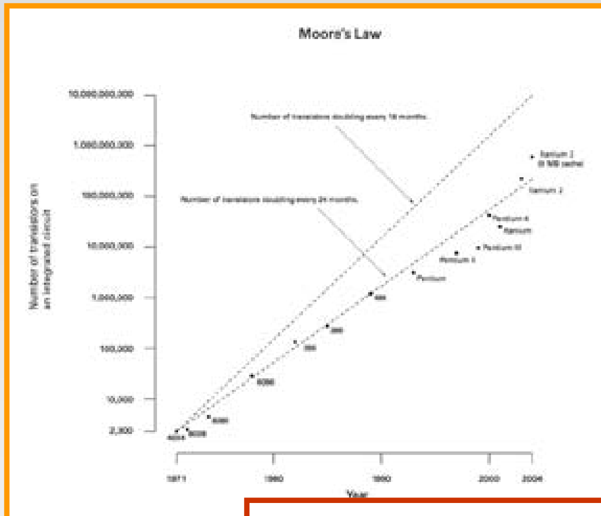
Computational Astrophysics Community

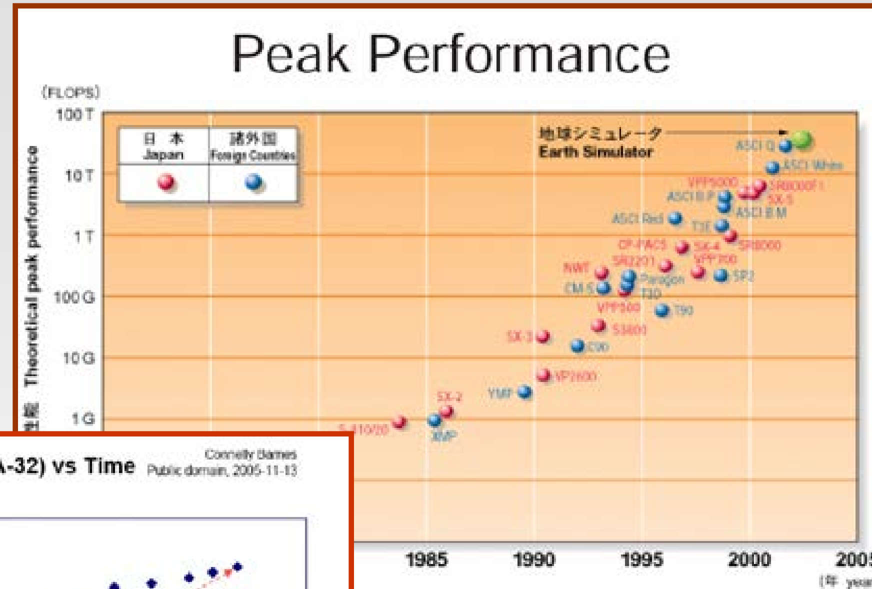
Funding level per group	small
Group size	small
Group expertise	limited
Number of groups	large
Project term	short
Intellectual property protection levels	high
Cross-verification abilities	low
Reusability factor	high
Discovery/funding prospects correlation	high

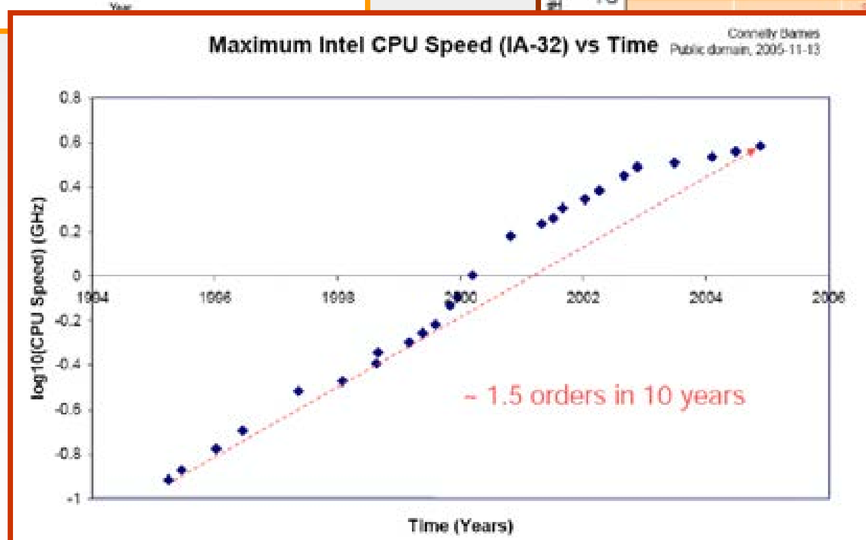
"Known knowns…"

- Steady improvements in **hardware** (processors, memory subsystems, data storage, networking, software).
- **Algorithmic** development (yields speedups comparable to hardware performance increase).
- Computer **implementation** development (single PE/cache efficiency, distributed memory communication, load balancing).
- Code **maintenance** and development system (cvs/svn/git, solution verification test suite).
- **Data analysis**-oriented (analytics) visualization (server-client model) and data storage system. Absolutely essential to complete production cycle!!

Benefits of Hardware Speedups…

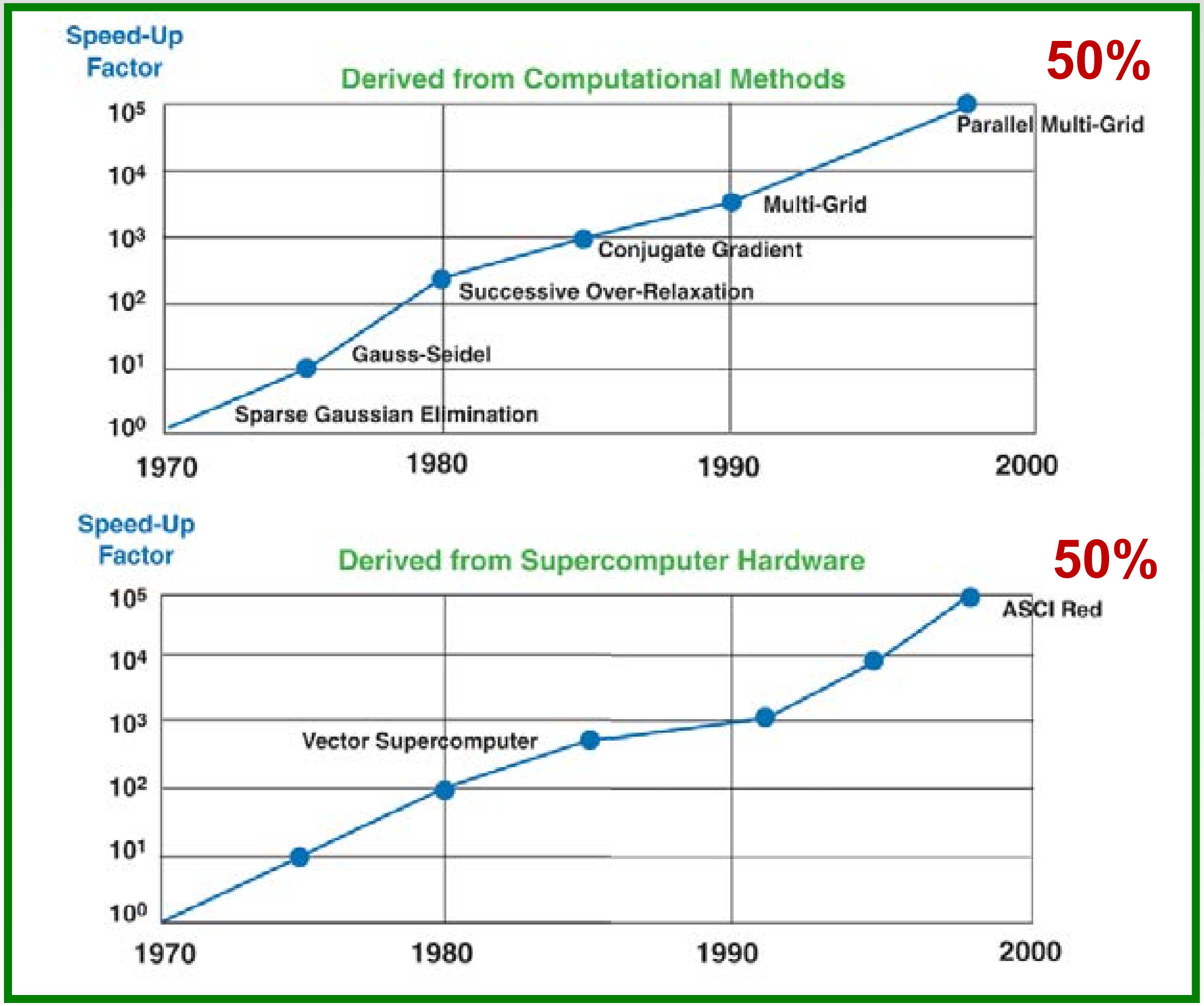






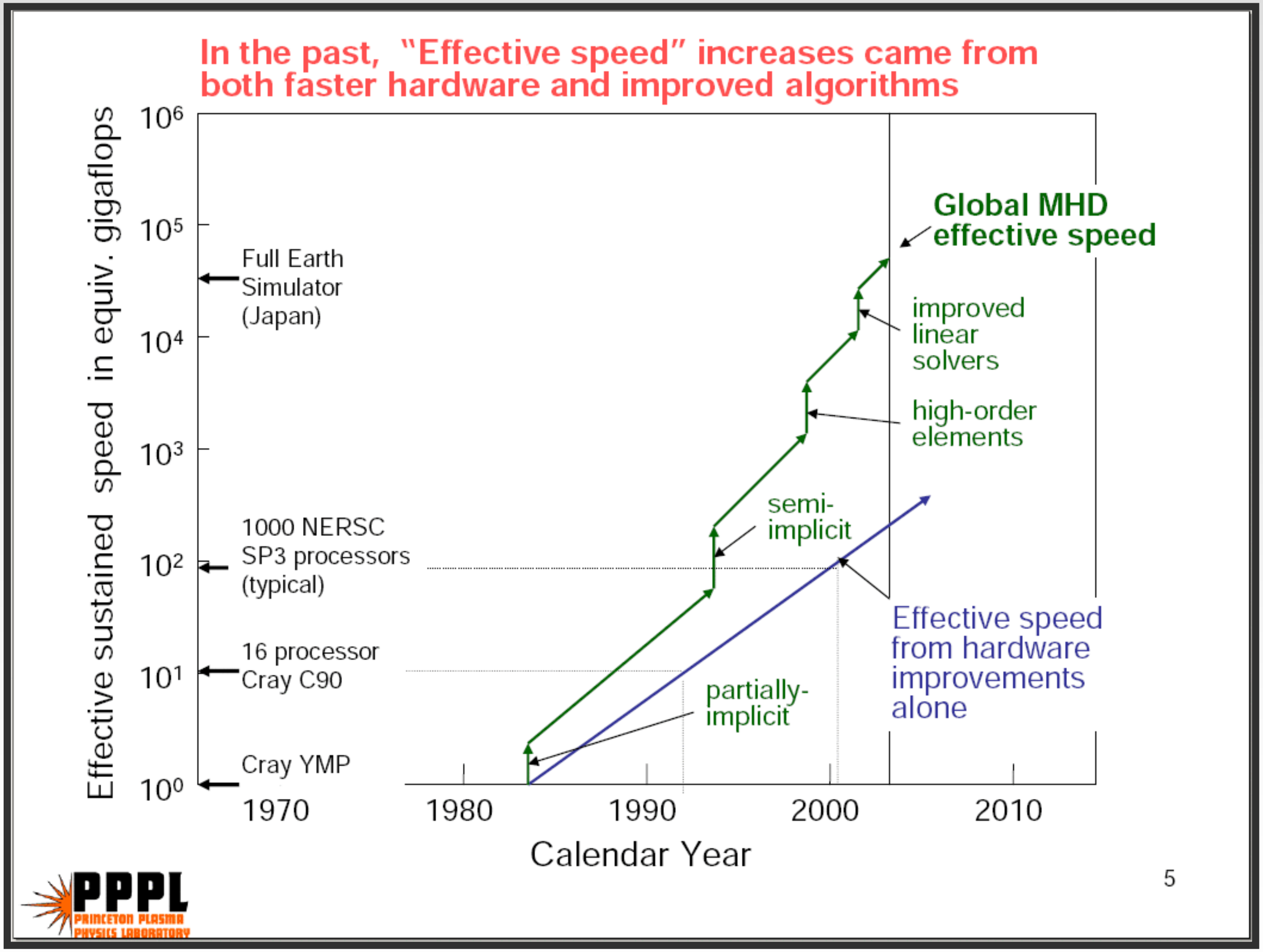
Barnes (2005)

…and Algorithmic Development



Petzold (2001)

Example: ITER Modeling



Jardin & Keyes (2006)

Algorithmic Gains Are Critical

How to get an additional 12 orders of magnitude in 10-15 years?

- 1.5 orders: increased parallelism
- 1.5 orders: processor speed and efficiency
- 4 orders: adaptive gridding
- 1 order: higher order elements
- 1 order: field-line following coordinates
- 3 orders: implicit algorithms

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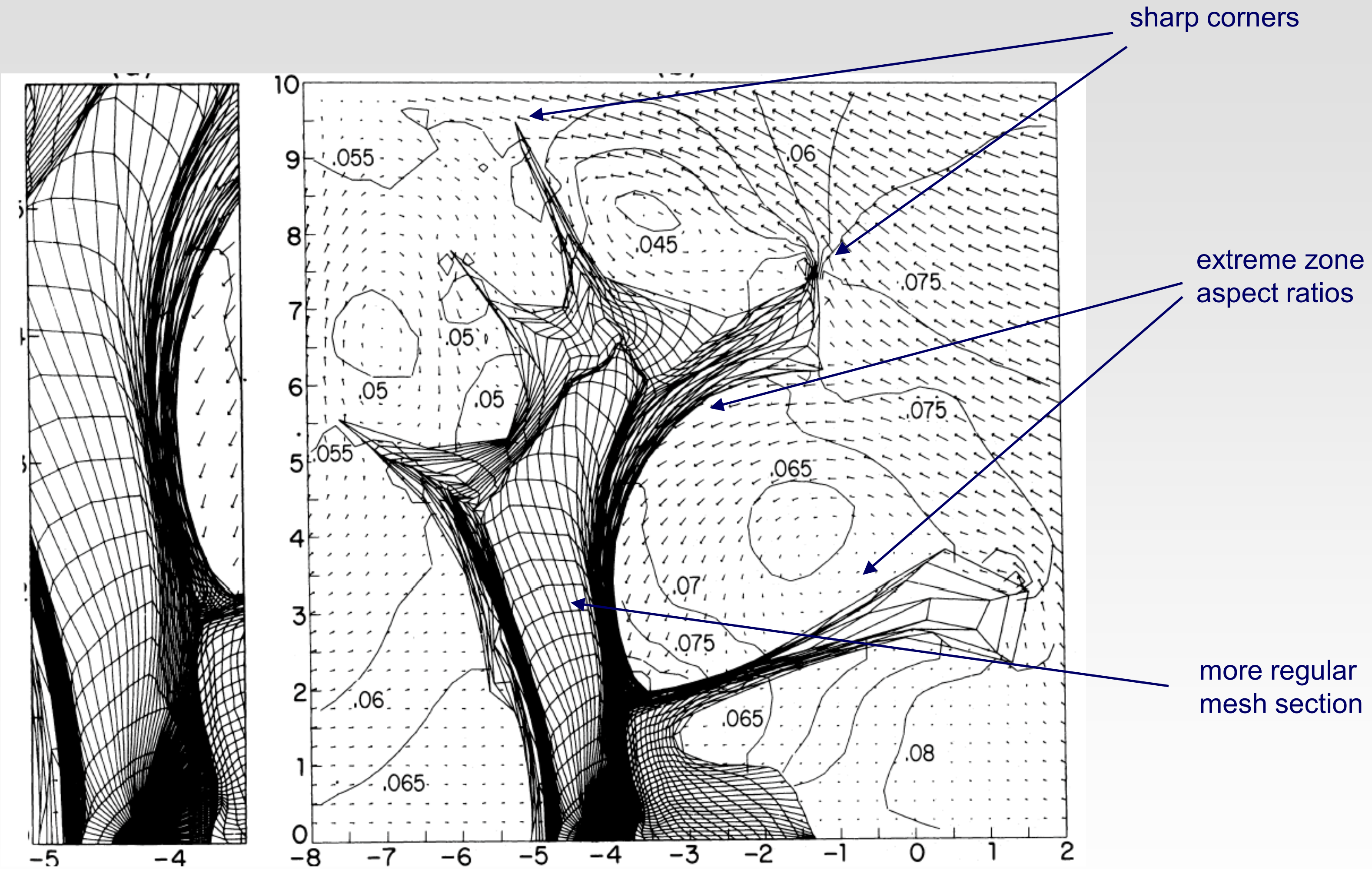
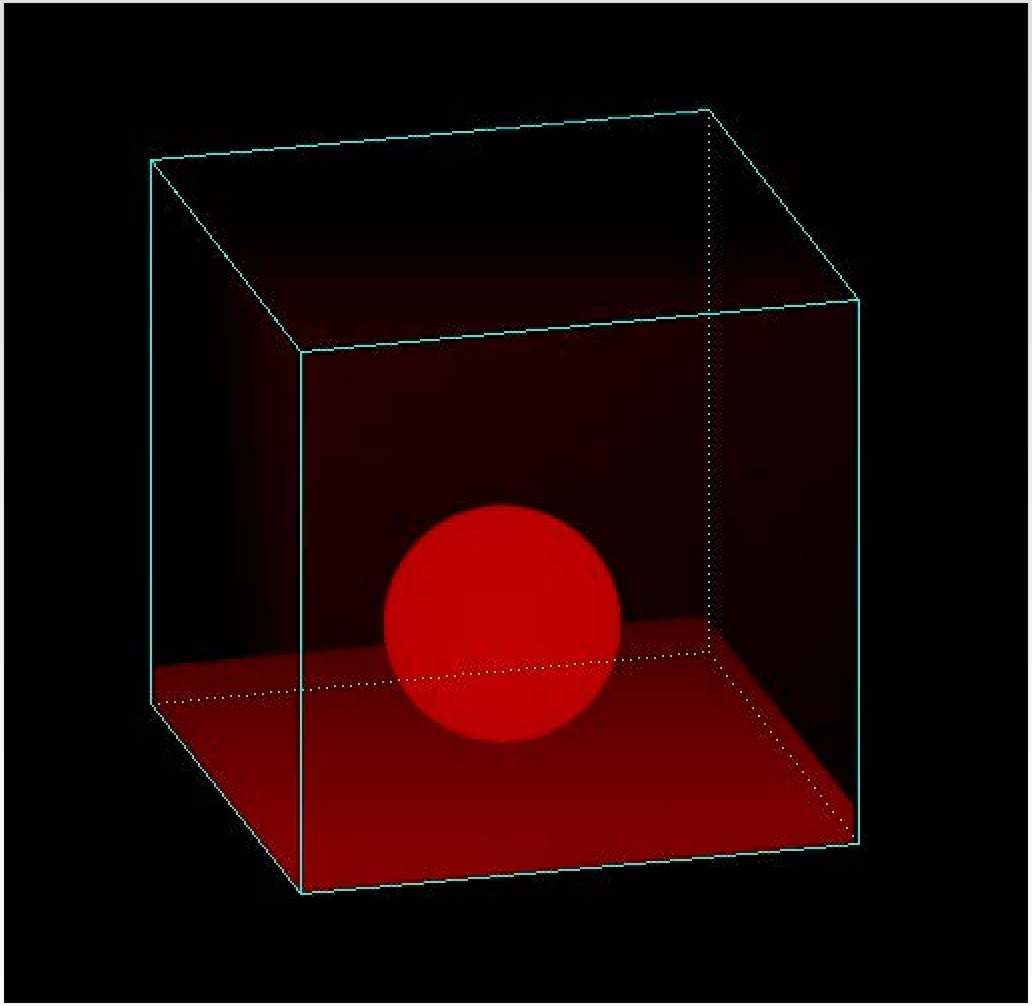
Jardin & Keyes (2006)

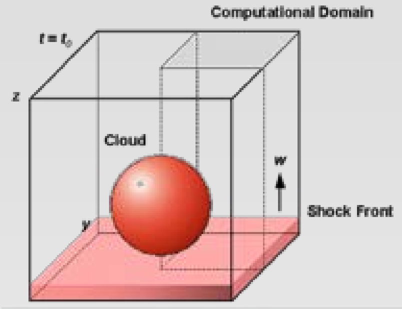
Improving algorithms in astrophysics



Woodward (1976)

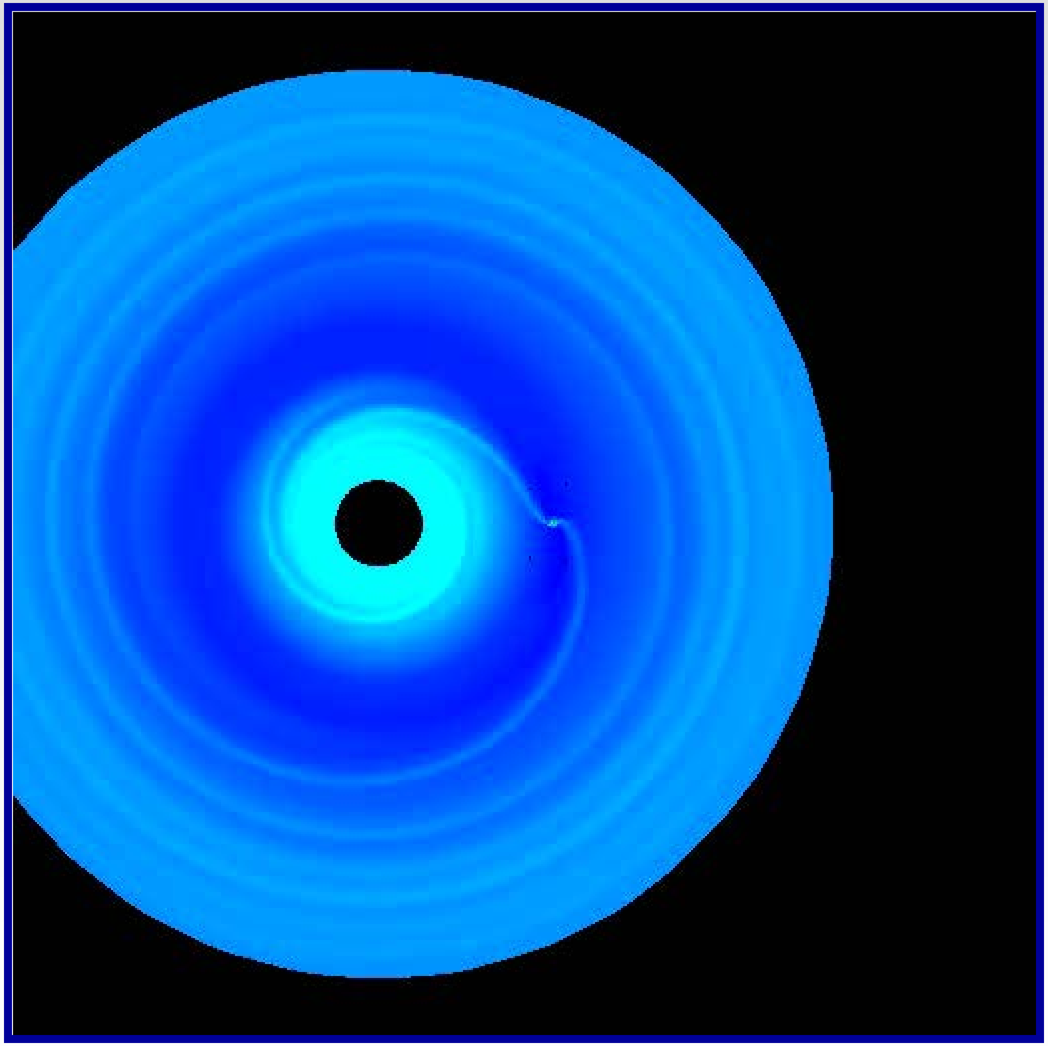
Eulerian AMR 3D Model

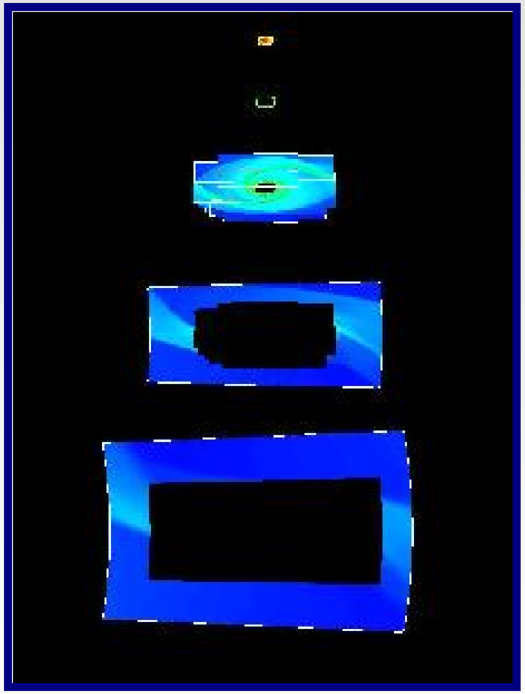




Orlando et al. (2006)

Adaptive Mesh Refinement





Fundamental Problem of Computational Science

We cannot redo most of the published computational results ourselves.

So how can we trust any of them???

“The real world is dangerous, Rapunzel!”

AKA “the need for being a responsible computational scientist.”

Main reasons for engineering disasters:

A. Modeling problem
   - The Tacoma Narrows Bridge
     (inadequate description of aerodynamical forces)
   - The Hartford Civic Center roof
     (inadequate linear model)
   - The Columbia Shuttle Accident
     (inadequate input data)

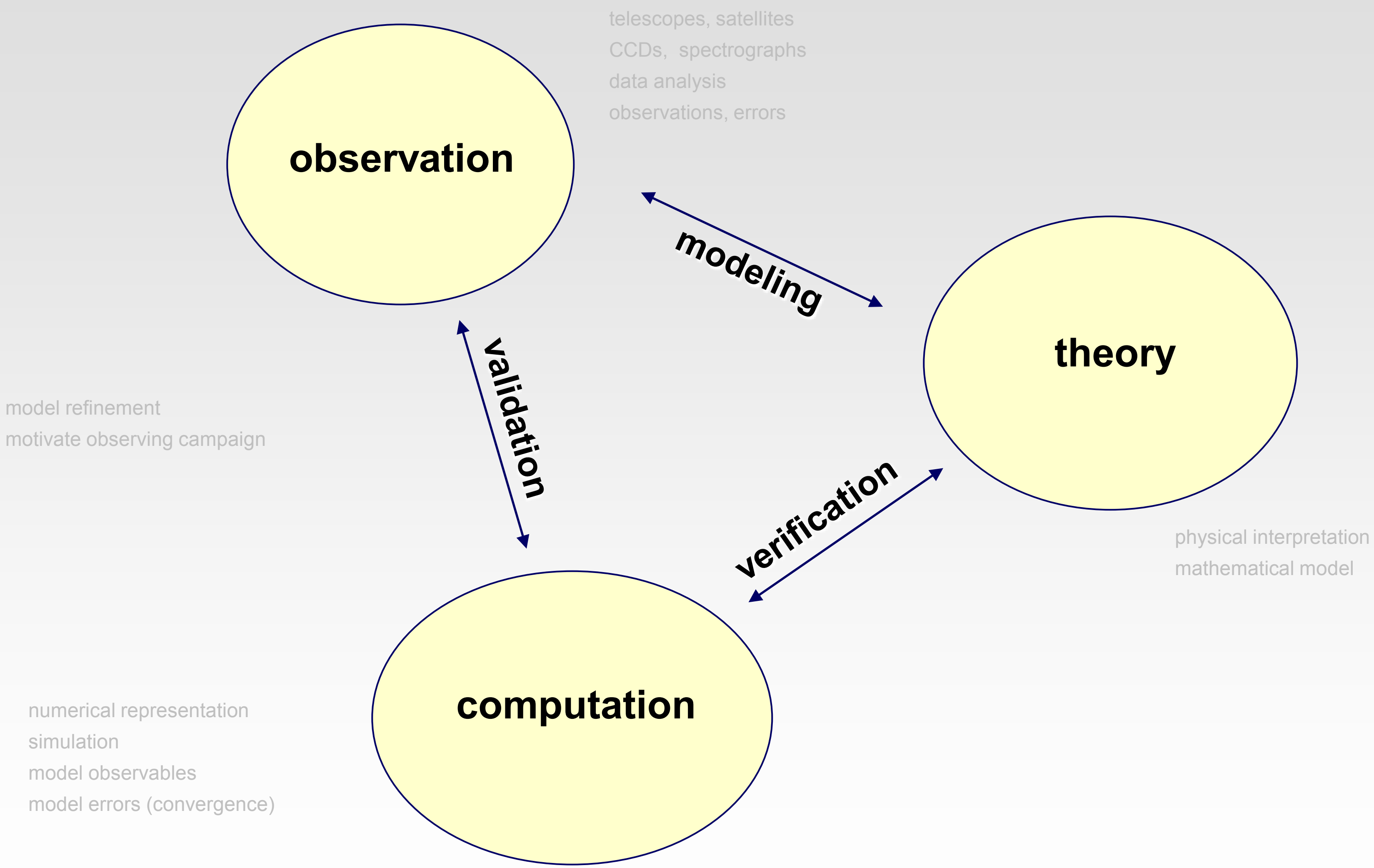
B. Numerical treatment problem
   - The Sleipner platform accident
     (FE analysis)

C. Computer Science problem
   - Ariane V rocket failure
     (roundoff errors)

D. Human error
   - Mars Climate Orbiter loss
     (SI/Imperial units mix)

After Babuska et al. (2007)

Activities


telescopes, satellites
CCDs, spectrographs
data analysis
observations, errors
observation
modeling
theory
validation
model refinement
motivate observing campaign
verification
physical interpretation
mathematical model
computation
numerical representation
simulation
model observables
model errors (convergence)

Code Verification

- **Code Verification:** *solving the equations right*

  Confirm that the software works as intended

  - **Software Quality Assurance (SQA)**
    - Software engineering
    - Static and dynamic testing
    - Done by code and model developer

Solution Verification

- **Solution Verification**

  Quantify the error of a numerical simulation by demonstration of convergence for the particular model under consideration, and, if possible, to provide an estimation of the numerical errors induced by the use of the model.

  - **Numerical error estimation**
    - Mathematical methods
    - Analytical solutions, benchmarks, manufactured solutions…
    - Grid convergence, time convergence
    - Model developer

Validation

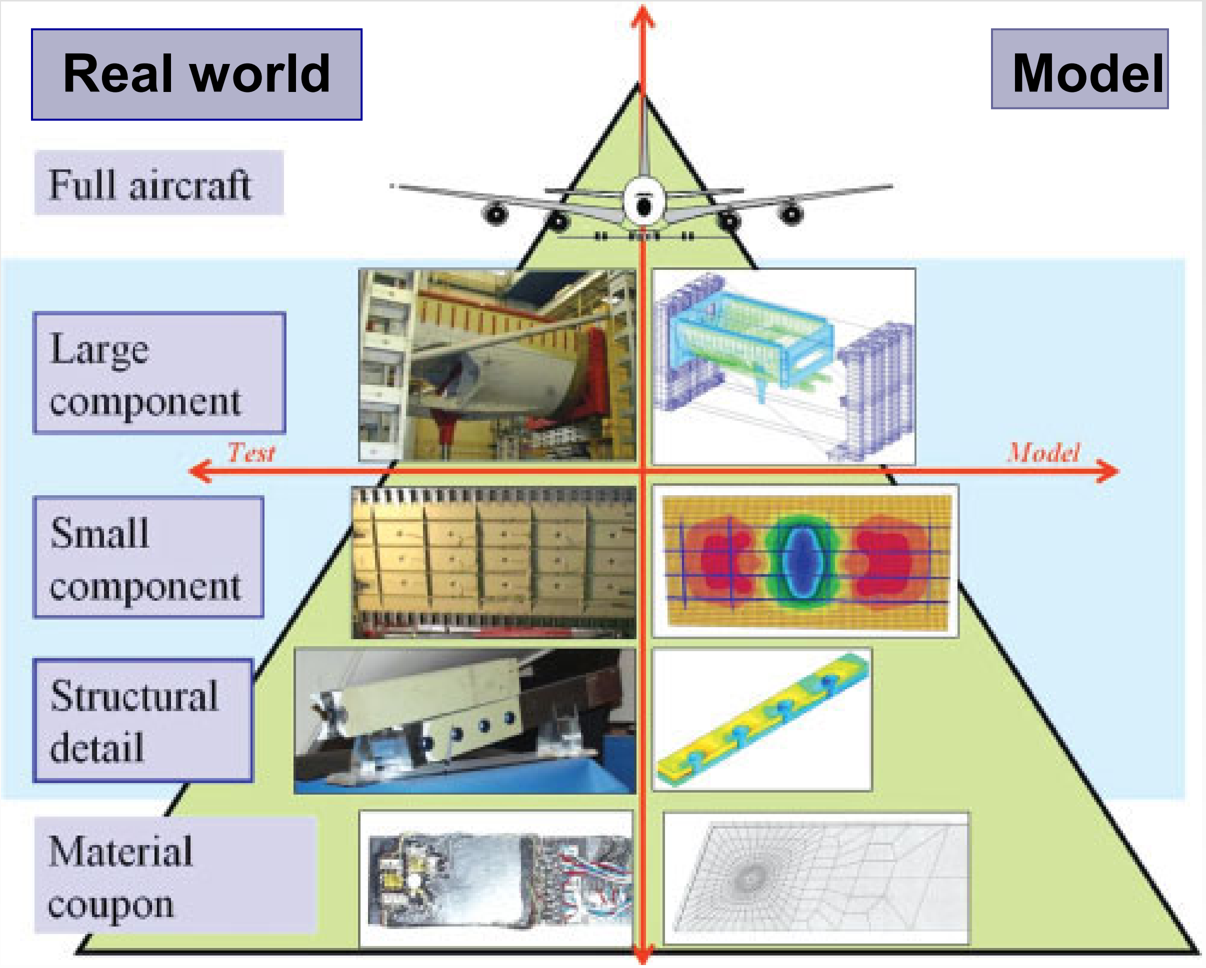
- **Validation:** *solving the right equations*

  Determine the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

> To **quantify confidence in the predictive capability** of the model by comparison with experimental data.

- **Prediction:** use of a model to foretell the state of a physical system for which the model has not been validated (*pushing the envelope*)

Validation Pyramid



Babuska et al. (2007)

Code is validated…

1. For a specific class of (nearby) problems
2. For specified variables
3. For a specified level of accuracy

No code can be totally validated!!

Experiments and Validation

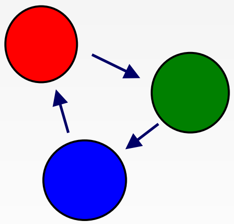
A conceptual model is needed prior to experimental data gathering.

- The experiment should be designed to exercise that conceptual model.
- Traditional experiments are designed to improve understanding of basic physics.

Not every experiment is a good validation experiment.

Code validation summary

- V&V is a **chain of procedures**
- The most scientifically attractive experiments are not necessarily good validation experiments**: need good validation experiments**
- **No code can be completely validated**
- Making next iteration: modifying experiments based on the simulation results => **closed feedback loop**



Uncertainty Quantification and Sensitivity Analysis

- **Verification**
  Involves error evaluation (calculation).

  Provides the error value.

- **Uncertainity Quanitification** (Richardson's extrapolation)
  Identify and characterize uncertainty in the model, i.e. not just values by the origin and character of, for example, errors in both inputs and outputs.

  Aleatory uncertainity: inherent randomness. Epistemic uncertainity: due to lack of knowledge.

- **Sensitivity Analysis** (sampling, automatic differentiation)
  How the variation in the input of a model impacts variation in the output of a model.

  Provides information on system response, trust regions, optimal regions, interactions between input parameters.

Typical SA/UQ Example #1

Sensitivity of p-process nucleosynthesis to nuclear reaction rates in a 25 M supernova model

Rapp, Görres, Wiescher, et al., 2006, ApJ, 653, 474

The astrophysical *p*-process, which is responsible for the origin of the proton-rich stable nuclei heavier than iron, was investigated using a full nuclear reaction network for a Type II supernova explosion when the shock front passes through the O/Ne layer. Calculations were performed with a multilayer model adopting the seed of a preexplosion evolution of a 25 *M* star. The reaction flux was calculated to determine the main reaction path and branching points responsible for synthesizing the proton-rich nuclei. In order to investigate the impact of nuclear reaction rates on the predicted *p*-process abundances, extensive simulations with different sets of collectively and individually modified neutron-, proton-, and -capture and photodisintegration rates have been performed. These results are not only relevant to explore the nuclear-physics-related uncertainties in *p*-process calculations but are also important for identifying the strategy and planning of future experiments.

Typical SA/UQ Example #2

On Variations in the Peak Luminosity of Type Ia Supernovae, Timmes, Brown, & Truran 2003, ApJ, 590, L83

We explore the idea that the observed variations in the peak luminosities of Type Ia supernovae (SNe Ia) originate in part from a scatter in metallicity of the main-sequence stars that become white dwarfs. Previous numerical studies have not self-consistently explored metallicities greater than solar. One-dimensional Chandrasekhar mass models of SNe Ia produce most of their ^{56}Ni in a burn to nuclear statistical equilibrium between the mass shells 0.2 and 0.8 M_{sun}, for which the electron-to-nucleon ratio Y_e is constant during the burn. We show analytically that under these conditions, charge and mass conservation constrain the mass of ^{56}Ni produced to depend *linearly* on the original metallicity of the white dwarf progenitor. Detailed postprocessing of W7-like models confirms this linear dependence. The effect that we have identified is most evident at metallicities larger than solar and is in agreement with previous self-consistent calculations over the metallicity range common to both calculations. The observed scatter in the metallicity (0.3 Z) of the solar neighborhood is enough to induce a 25% variation in the mass of ^{56}Ni ejected by SNe Ia. This is sufficient to vary the peak *V*-band brightness by $|M_V|$~0.2. […]

V&V, SA and UQ in Astrophysics

- **Verification** uses analytic solutions; (self-)convergence studies done almost exclusively in spatial domain
- **Code-to-code comparisons** since late1980s; several projects later; growing in popularity (self-confidence builders)
- **Validation largely limited** to “application of astrophysics code to experiment”
- Historically **more emphasis on observations** rather than laboratory experiments
- **Real UQ/SA is mostly absent** due to high “added” cost (discovery is valued much higher)

The Seven Deadly Sins of Verification

1. Assume the code is correct.
2. Providing only a qualitative comparison.
3. Use of problem-specific settings.
4. Code-to-code comparison only.
5. Computing on one mesh only.
6. Show only results that make the code "look good".
7. Don't differentiate between accuracy and robustness.

by Bill Rider (as quoted by Jim Kamm)

References

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- Frenk, C. S., White, S. D. M., Bode, P., et al. 1999, ApJ, 525, 554
- de Val-Borro, M., Edgar, R.G., Artymowicz, P., et al. 2006, MNRAS, 370, 529
- Liebendörfer, M., Rampp, M., Janka, H.-Th., & Mezzacappa, A. 2005, ApJ, 620, 840