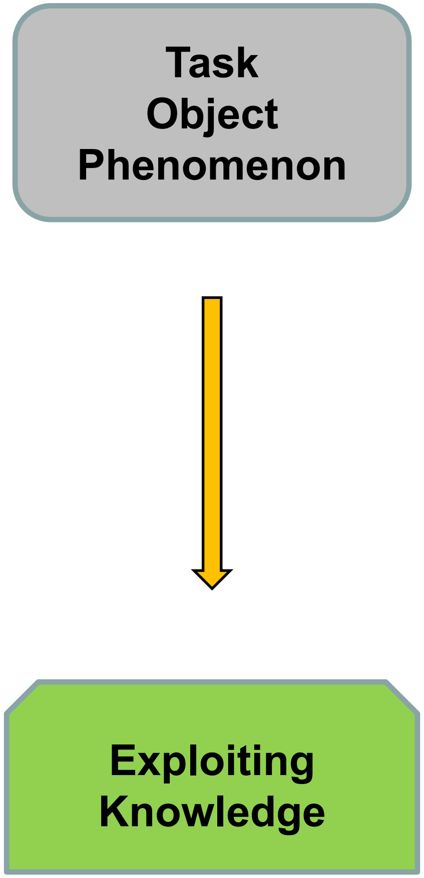
Numerical Experiment

Vasily Arzhanov

Reactor Physics, KTH

Why Do We Do Calculations?

Improving Quality of Life



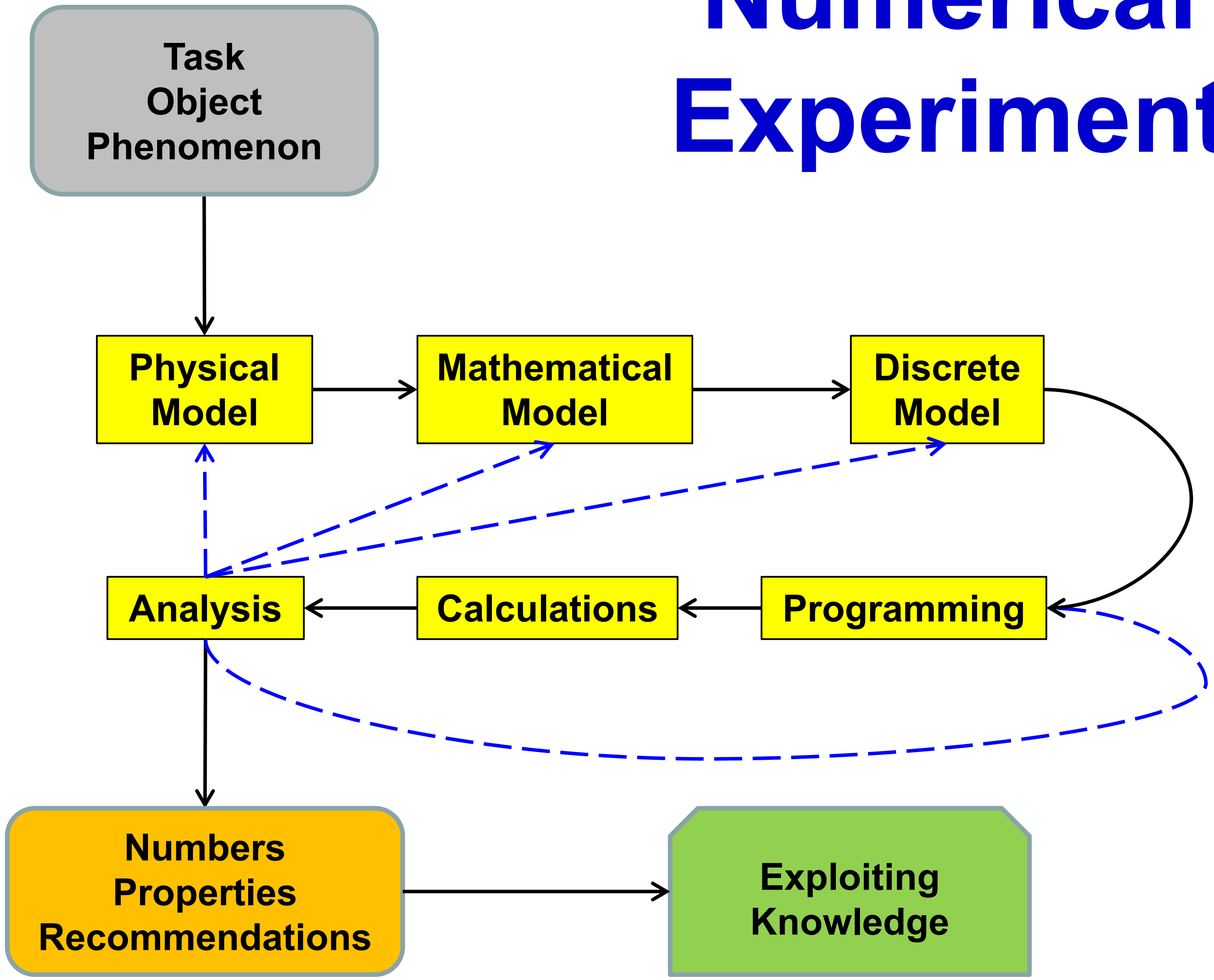
Nuclear Power in Sweden

- 1947, Atomic Energy Company
- 1954, First small research HWR
- 1964, 2 HWRs in Ågesta and Marviken
- 1968, Non-Proliferation Treaty
- 1970s, 6 commercial nuclear reactors
- 1980s, 6 commercial nuclear reactors
- Design: 9 by ASEA, 3 by Westinghouse

Nuclear Policy in Sweden

- 1980, Government to phase out by 2010
- Several units are closed in 1999 and 2005
- Currently 3 power plants (40 – 50%)
  - Forsmark: 3 BWRs
  - Oskarshamn: 1 BWR
  - Ringhals: 2 PWRs
- 2009 Feb 9, Gvmt replacement policy

Numerical Experiment

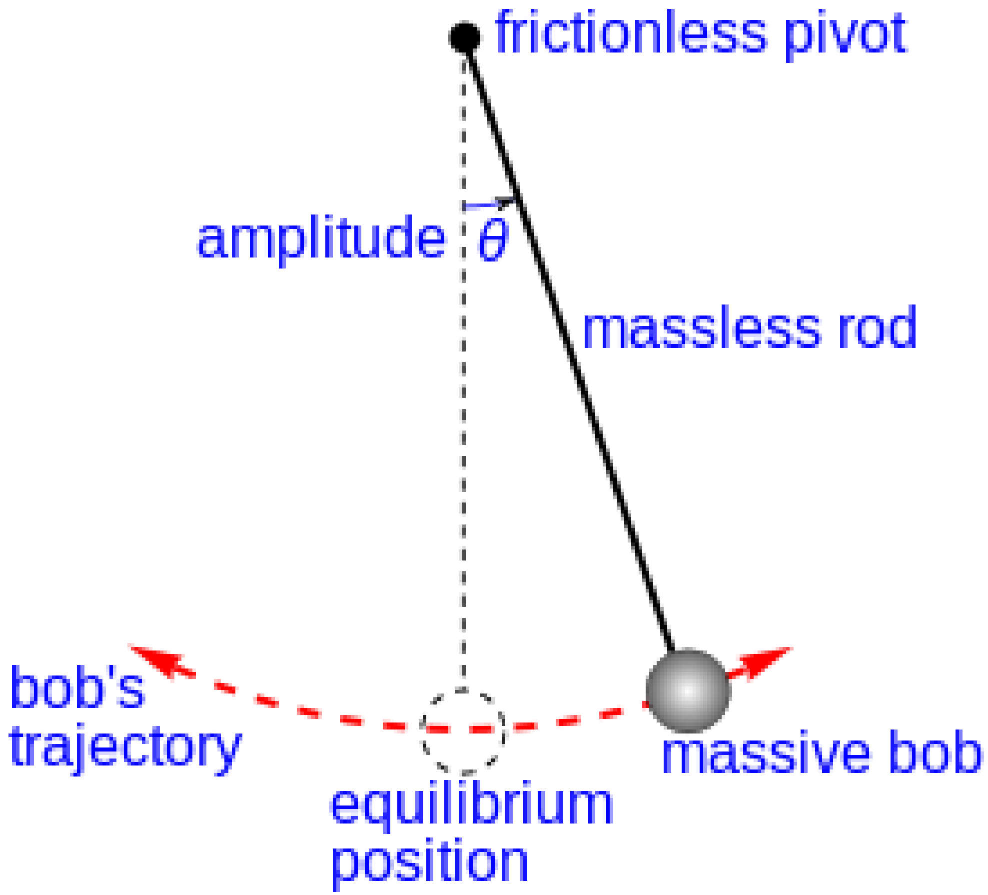


Physical Model

A framework of ideas and concepts from which we interpret our observations and experimental results.

- Set of Natural Laws
- List of Relevant Physical Phenomena
- List of Irrelevant Physical Phenomena
- Set of Ideal Physical Objects
- Definitions of Relevant Physical Quantities

Physical Model



Mathematical Model

- Definition of Mathematical Quantities
- List of Mathematical Equations
- Approximations
- Limitations
- Area of Validity

Mathematical Model, cont

$$l\frac{d^2\theta}{dt^2} + g \cdot \sin\theta = 0$$

$$l\frac{d^2\theta}{dt^2} + g \cdot \theta = 0$$

Discrete Model

- Discretisation (of Regions and Functions)
- Reduction to Discrete Equations
- Convergence to Original Equations
- Approximation Error
- Solution Method (typically iterative)
- Iteration Convergence, Error

Discrete Model, cont

$$\left[0,T\right] \longrightarrow \left[t_0, t_1, \ldots t_N\right] \qquad t_i = i \cdot h \qquad h = \frac{T}{N}$$

$$l\frac{d^2\theta}{dt^2} + g \cdot \sin\theta = 0$$

$$l\frac{\theta_{i+1} - 2\theta_i + \theta_{i-1}}{h^2} + g \cdot \sin\theta_i = 0$$

Programming

- Algorithm
- Representation of Initial Data
- Representation of Output Data
- Programming Model (Procedural, OOP)
- Data Objects
- Verification (debugging)

Calculation

- Exceptional Events
- Divergence
- Unexpected Behaviour
- Representation of Results
  - Numbers
  - Tables
  - Plots
  - Visualisation

Analysis

- Verification
- Validation
- Knowledge

Remember:

- ➢ Any serious numerical project involves serious analytic work
- ➢ Many equations come from physics
- ➢ Many equations in physics reflect conservational laws
- ➢ Physical dimensions are important
- ➢ Scaling is important

Original Equation

$$-D\phi''(x) + \Sigma_a \phi(x) = S(x)$$

$$D\left[\mathrm{cm}\right] \quad \Sigma_a\left[\mathrm{cm}^{-1}\right]$$

Order of Magnitude

$$-D\phi''(x) + \Sigma_a \phi(x) = S(x)$$

$$S \sim 10^6 \div 10^{16} \left[\frac{\mathrm{n}}{\mathrm{s}}\right], \qquad \phi \sim 10^8 \div 10^{18} \left[\frac{\mathrm{n}}{\mathrm{cm}^2\mathrm{s}}\right].$$

Scaling Dependent Variable

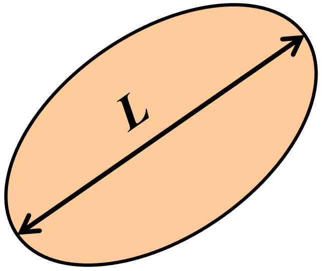
$$-D\phi''(x)+\Sigma_a\phi(x)=S(x) \qquad \phi(x)\sim 10^{8}\div 10^{18}$$

$$\phi_{\mathrm{SF}}\equiv 10^{12}\left[\frac{\mathrm{n}}{\mathrm{cm^2 s}}\right] \qquad \Phi(x)\equiv\frac{\phi(x)}{\phi_{\mathrm{SF}}} \qquad Q(x)\equiv S(x)/\phi_{\mathrm{SF}}$$

$$-D\Phi''(x)+\Sigma_a\Phi(x)=Q(x) \qquad \Phi(x)\sim 1$$

Scaling Independent Variable

$$-D\Phi''(x) + \Sigma_a \Phi(x) = Q(x)$$



$$z \equiv x/L \qquad x \equiv Lz$$

$$\psi(z) \equiv \Phi(Lz) \longrightarrow \frac{d\psi(z)}{dz} = \frac{d\Phi(x)}{dx} \cdot \frac{dx(z)}{dz}$$

$$\psi'(z) = \Phi'_x(Lz) \cdot L \qquad \psi''(z) = \Phi''_{xx}(Lz) \cdot L^2 \qquad \Phi''_{xx}(x) = \frac{1}{L^2}\psi''(z)$$

$$-\psi''(z) + \frac{L^2 \Sigma_a}{D}\psi(z) = q(z) \equiv \frac{L^2}{D} Q(Lz)$$

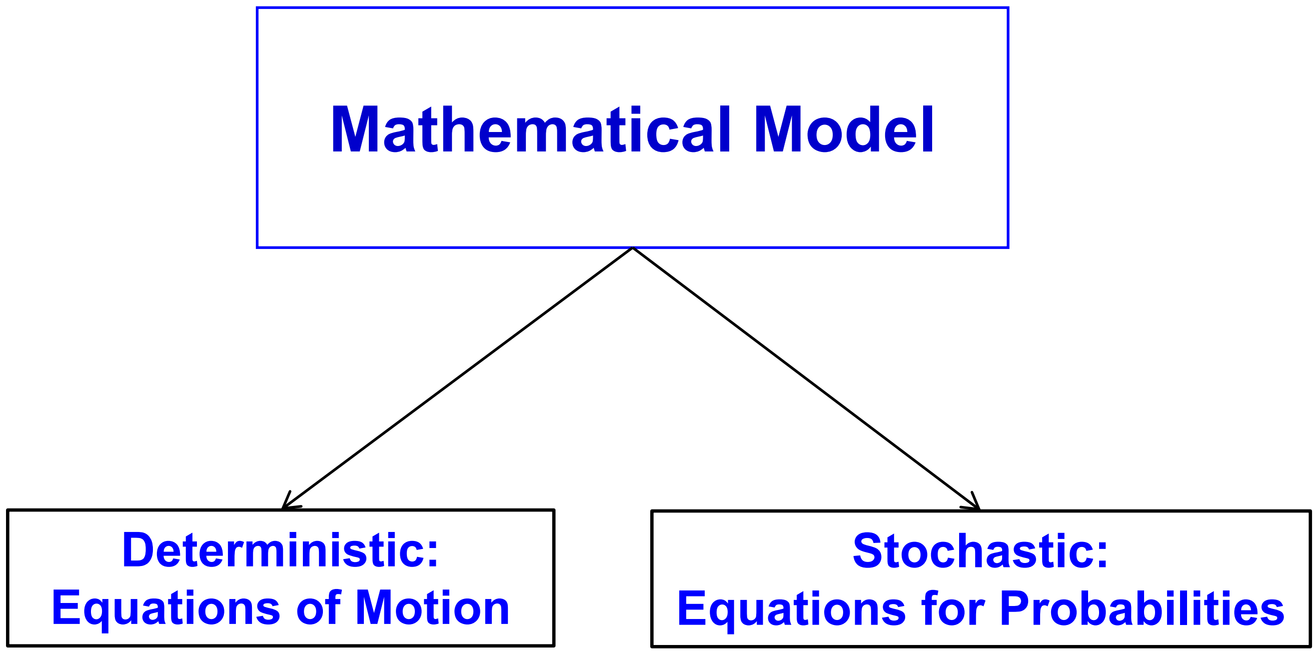
Smart Scaling

$$-\psi''(z) + \frac{L^2\Sigma_a}{D}\psi(z) = q(z) \equiv \frac{L^2}{D}Q(Lz)$$

$$L^2 \equiv \frac{D}{\Sigma_a} \longrightarrow \frac{L^2\Sigma_a}{D} = 1$$

$$-\psi''(z) + \psi(z) = q(z)$$

Deterministic vs. Stochastic



(Numerical Methods)

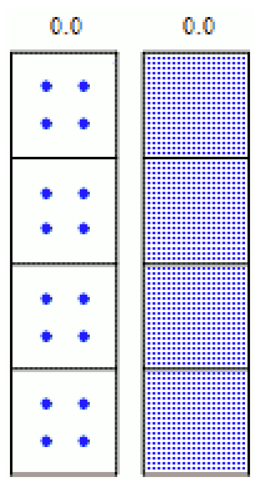
(Monte Carlo Methods)

Radioactivity Law

- A nuclear decay is a spontaneous quantum transformation.
- The exact time of a decay cannot be predicted.
- The decrease in the number of nuclei is proportional to the number of nuclei present and the time interval

Deterministic: $-dn = \lambda \cdot n \cdot dt \longrightarrow \dfrac{dn}{dt} = -\lambda n \longrightarrow n(t) = n(0)\, e^{-\lambda t}$

Stochastic:



Free neutrons:

$$\bar{t} = 885.7 \text{ sec} \;=\; 14 \text{ min } 45.7 \text{ sec}$$

$$T_{1/2} = 613.9 \text{ sec} \;=\; 10 \text{ min } 13.9 \text{ sec}$$

Well-Posed Problems

$$F(x,d)=0$$

Jacques Salomon Hadamard (1865-1963); 1923:

1) A solution exists
2) The solution is unique
3) The solution depends continuously on data

Ill-Posed Problems

$$F(x,d)=0$$

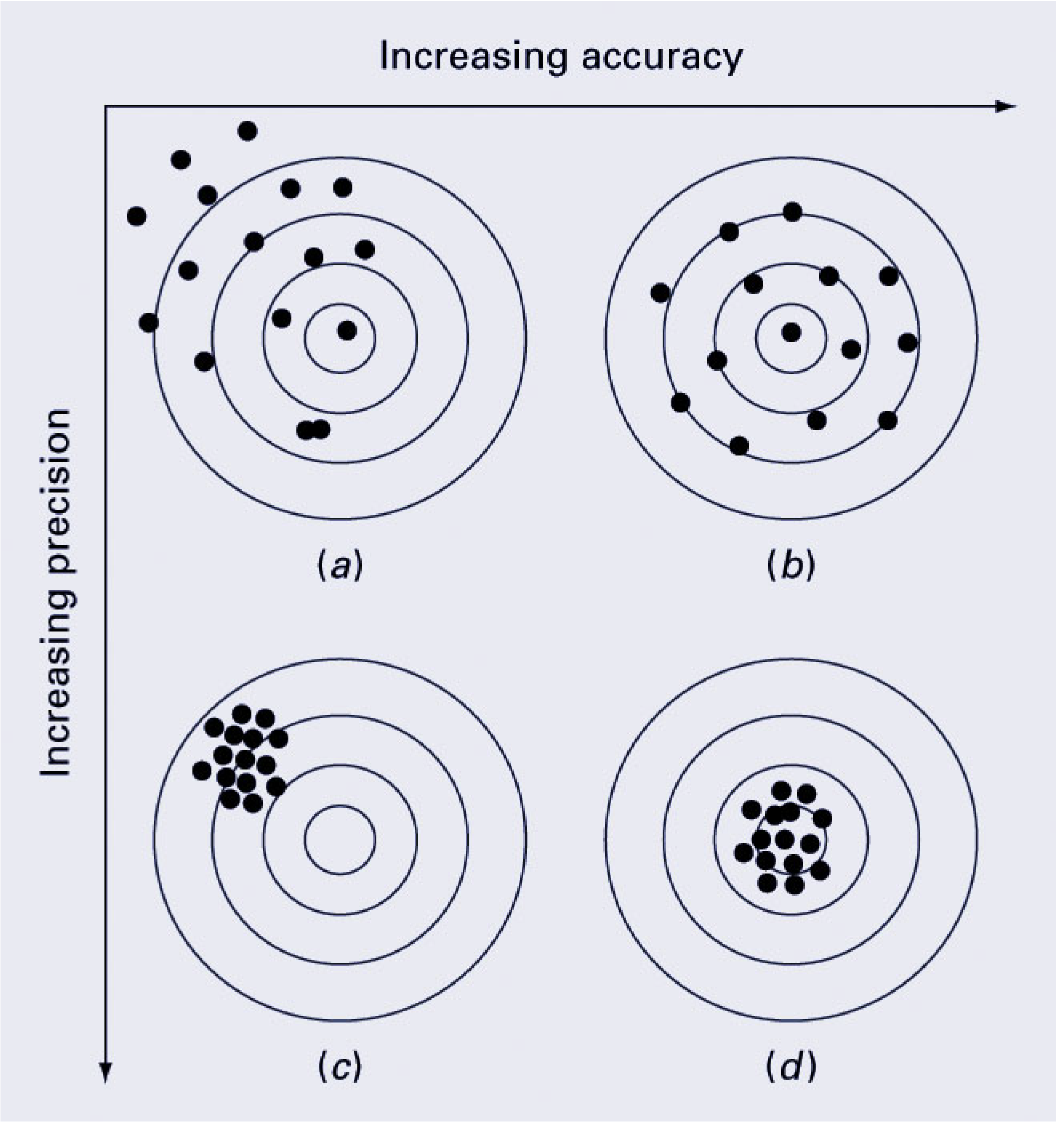
Andrei Tikhonov (1906-1993)

Regularization method to solve ill-posed

- Pattern recognition
- Inverse diffusion problem (finding previous temperature distribution)

Accuracy vs. Precision

- Joint Committee for Guides in Metrology "International Vocabulary of Metrology, VIM, Basic and General Concepts and associated Terms", JCGM 200:2008.
- Accuracy refers to how closely a computed or measured value agrees with the true value.
- Precision refers to how closely individual measurements or computed values agree with each other.


Increasing accuracy
Increasing precision
(a)
(b)
(c)
(d)

Existence and Uniqueness

$$S = 1 + 2 + 2^2 + 2^3 + \ldots$$

$$2S = 2 + 2^2 + 2^3 + \ldots$$

$$1 + 2S = 1 + 2 + 2^2 + 2^3 + \ldots = S$$

$$S = -1$$

Importance of Good Notation

Scipione del Ferro, 1465 – 1526.

$$x^3 + mx = n \quad \Rightarrow \quad x = \sqrt[3]{\frac{n}{2} + \sqrt{\frac{n^2}{4} + \frac{m^3}{27}}} - \sqrt[3]{-\frac{n}{2} + \sqrt{\frac{n^2}{4} + \frac{m^3}{27}}}$$

Cube one-third the coefficient of *x*; add to it the square of one-half the constant of the equation; and take the square root of the whole. You will duplicate this, and to one of the two you add one-half the number you have already squared and from the other you subtract one-half the same... Then, subtracting the cube root of the first from the cube root of the second, the remainder which is left is the value of *x* (Gerolamo Cardano, *Ars Magna*, 1545).

Important

- Concept of Numerical Experiment
- Scaling
- Two Kinds of Mathematical Models
  - Deterministic
  - Stochastic
- Well-Posed/Ill-Posed Problems
- Accuracy and Precision
- Verification and Validation