Principles of MATHEMATICAL MODELING

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Why Modeling?

- Fundamental and quantitative way to understand and analyze complex systems and phenomena
- Complement to Theory and Experiments, and often Intergate them
- Becoming widespread in: Computational Physics, Chemistry, Mechanics, Materials, …, Biology

What are the goals of Modeling studies?

- Appreciation of broad use of modeling
- Hands-on an experience with simulation techniques
- Develop communication skills working with practicing professionals

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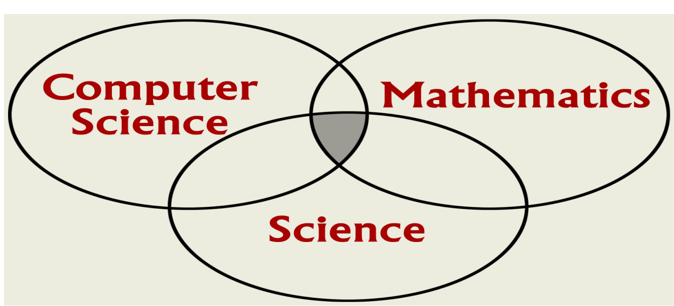
Mathematical Modeling?

Mathematical modeling seeks to gain an understanding of science through the use of mathematical models on HP computers.



Mathematical modeling involves teamwork

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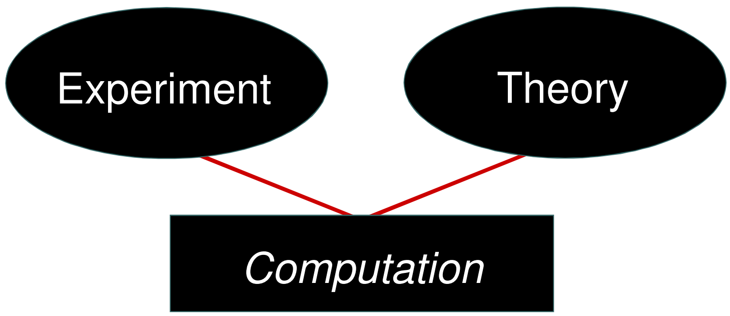
Mathematical Modeling

Complements, but does not replace, theory and experimentation in scientific research.



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Mathematical Modeling

- Is often used in place of experiments when experiments are *too large, too expensive, too dangerous, or too time consuming*.
- Can be useful in “what if” studies; e.g. to investigate the use of *pathogens* (viruses, bacteria) to control an insect population.
- Is a modern tool for *scientific investigation.*

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Mathematical Modeling

Has emerged as a powerful, indispensable tool for studying a variety of problems in scientific research, product and process development, and manufacturing.

- Geosciences
- Petroleum and Gas
- Seismology
- Climate modeling
- Economics
- Environment
- Material research
- Drug design
- Manufacturing
- Medicine
- Biology

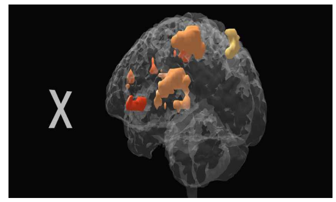
Analyze - Predict

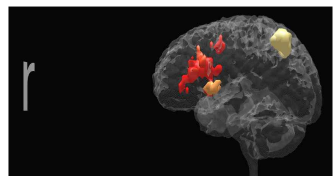
Example: Industry →

- First jetliner to be digitally designed, "pre-assembled" on computer, eliminating need for costly, full-scale mockup.
- Computational modeling improved the quality of work and reduced changes, errors, and rework.

Example: Roadmaps of the Human Brain

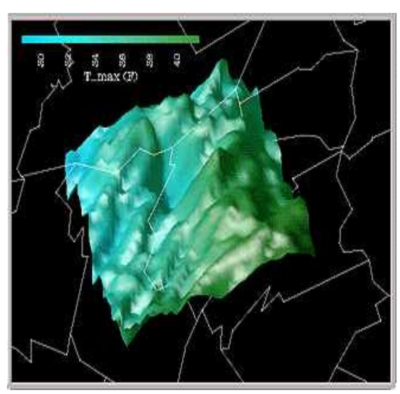
- Cortical regions activated as a subject remembers the letters x and r.
- Real-time Magnetic Resonance Imaging (MRI) techno-logy may soon be incorporated into dedicated hardware bundled with MRI scanners allowing the use of MRI in drug evaluation, psychiatry, & neurosurgical planning.



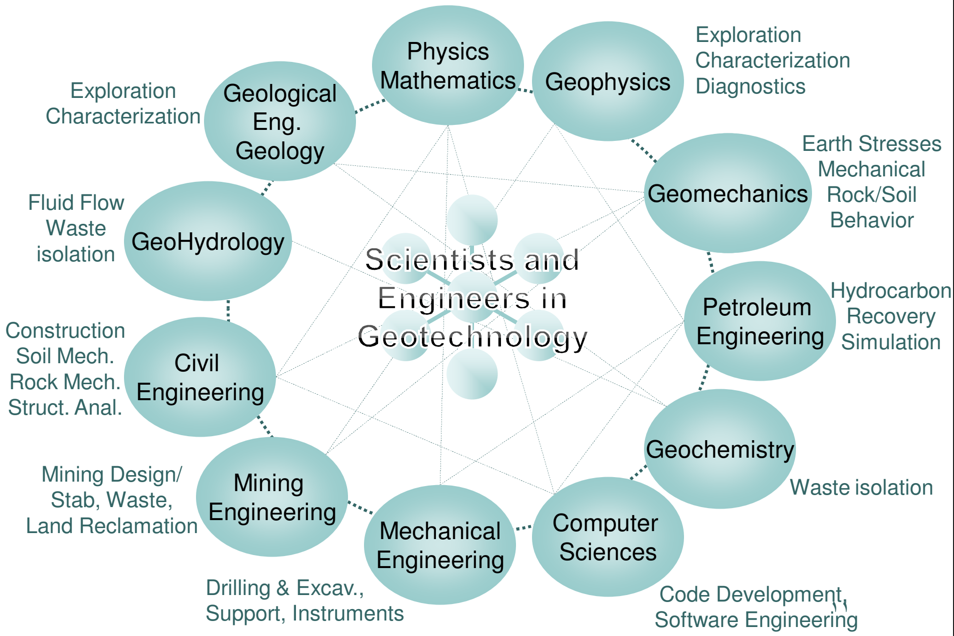


Example: Climate Modeling

- 3-D shaded relief representation of a portion of PA using color to show max daily temperatures.
- Displaying multiple data sets at once helps users quickly explore and analyze their data.

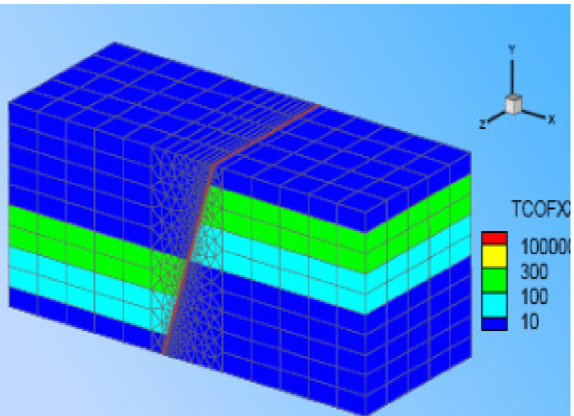


Highly Integrated
Multidisciplinary, Multiscale, Multiprocess

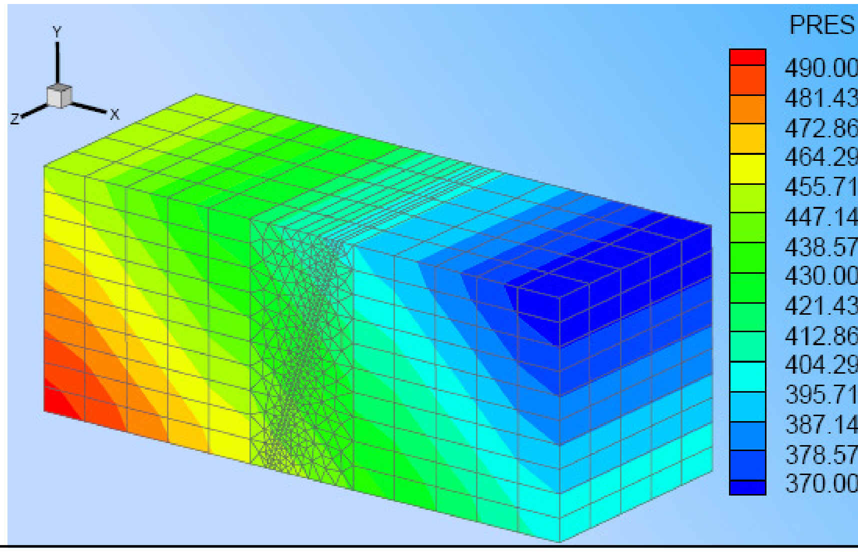


FD & FEM Couplings: 3 Blocks with Fault

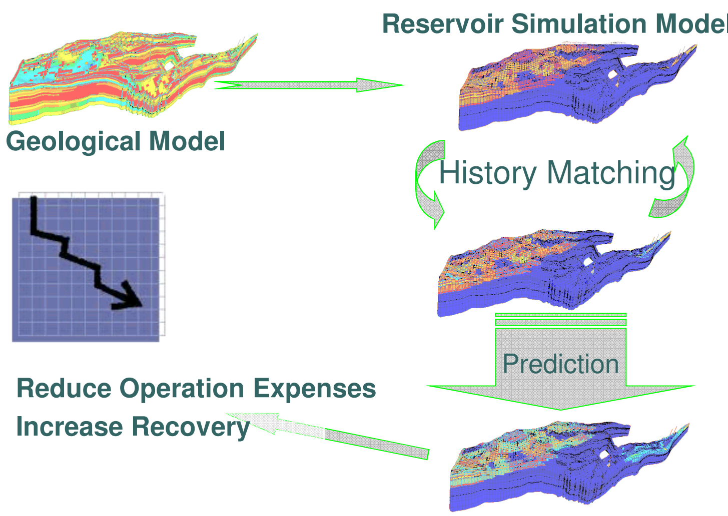
- $250 \times 100 \times 100$ ft
- 2 ft wide fault: 10000 mD, $\phi = 0.01$
- 4 geological layers: 10, 100, 300, 10 mD, $\phi = 0.2$
- BC:
  500 psi at $x = 0$,
  400 psi at $x = 250$,
  noflow o.w.
- $r = 2, k = 0(RT_0), m = 0$



Solution

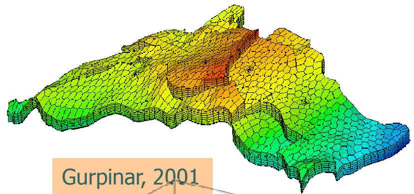


Prediction Future performance

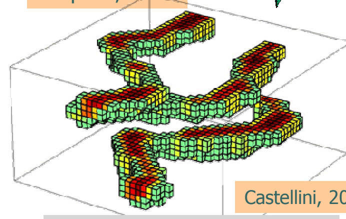


Gridding

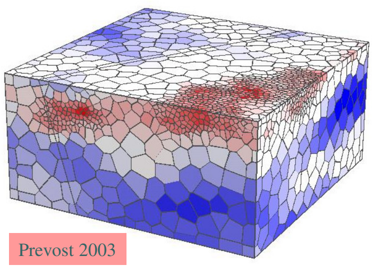
- Honor geology
- Preserve numerical accuracy
- Be easy to generate



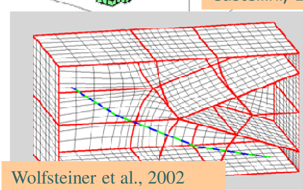
Gurpinar, 2001



Castellini, 2001



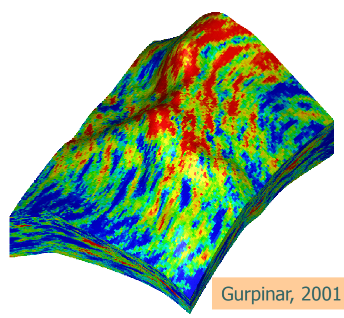
Prevost 2003



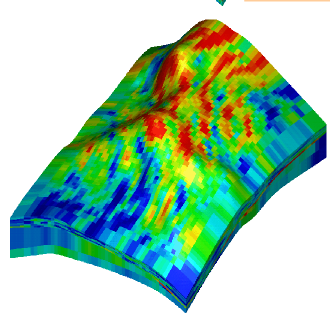
Wolfsteiner et al., 2002

Upscaling

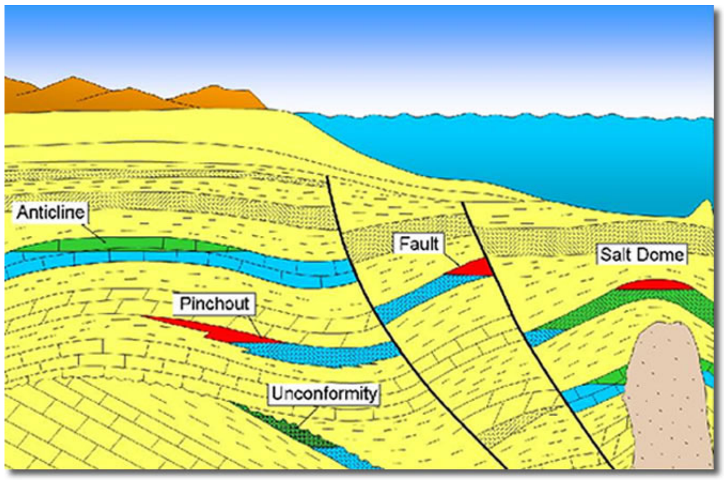
- Optimum level of and techniques for upscaling to minimize errors



Gurpinar, 2001



Geology



www.lonestarsecurities.com

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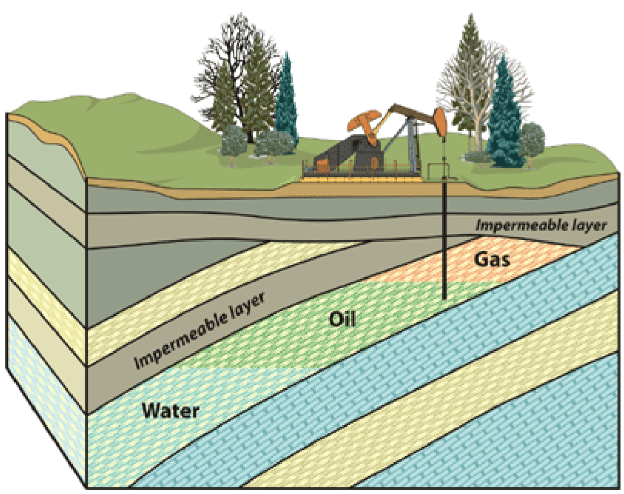
Oil and Gas Reservoir



www.geoscape.nrcan.gc.ca

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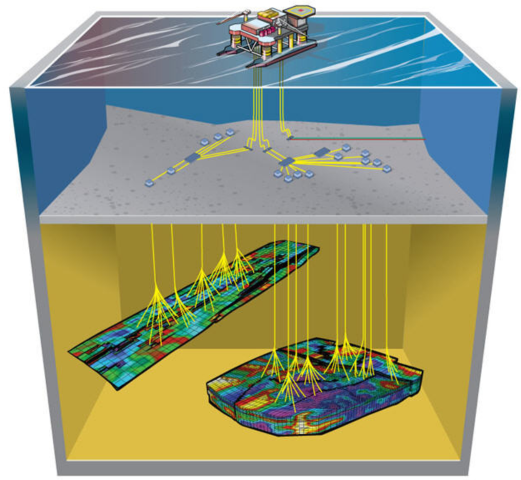
Petroleum Reservoir Modeling



www.halliburton.com

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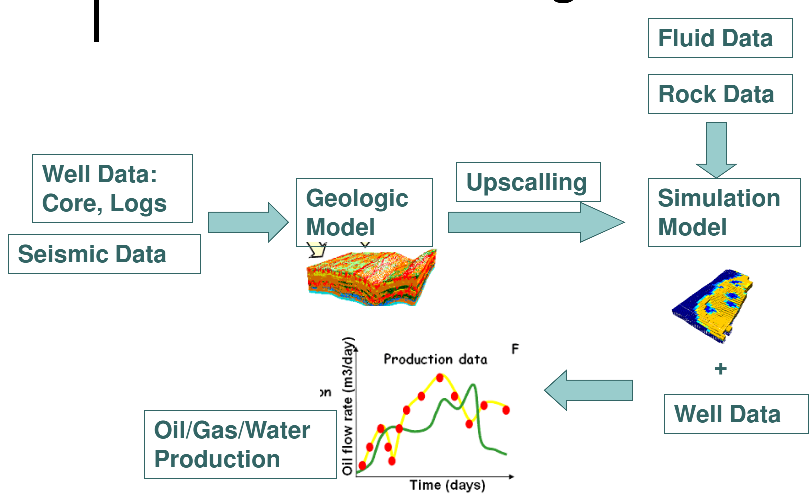
Reservoir Modeling Process



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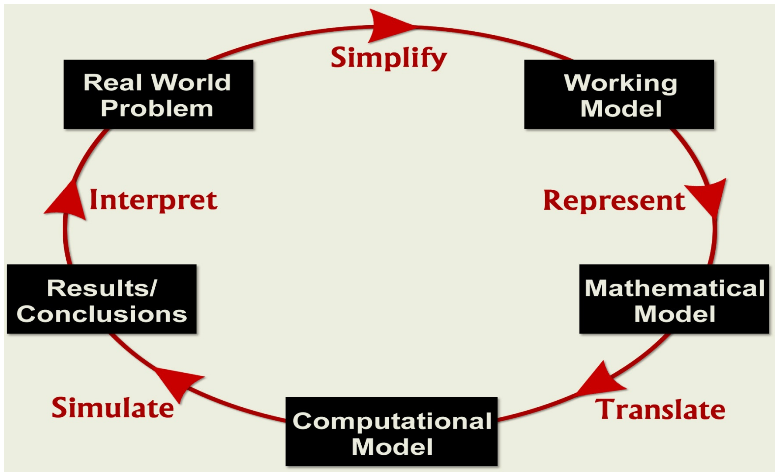
Mathematical Modeling Process



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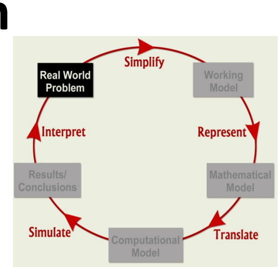
Real World Problem



Identify *Real-World Problem*:

- Perform background research, focus on a workable problem.
- Conduct investigations (Labs), appropriate.
- Learn the use of a computational tool: Maple, Matlab, Mathematica, Excel, Java.

Understand current activity and predict future behavior.

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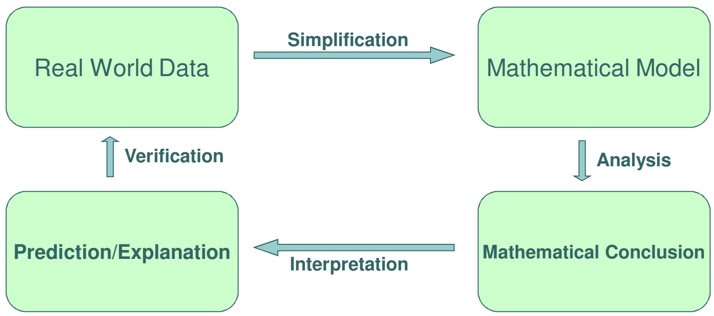
Modeling Process



Example: Falling Rock

Determine the motion of a rock dropped from height, H, above the ground with initial velocity, V.

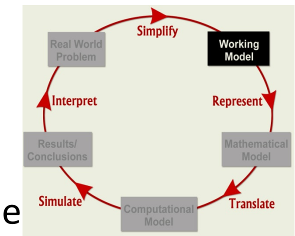
A *discrete model*: Find the position and velocity of the rock above the ground at the equally spaced times, t0, t1, t2, …; e.g. t0 = 0 sec., t1 = 1 sec., t2 = 2 sec., etc.

|_____|_____|__________|_____ >

t0 t1 t2 … tn

Working Model

Simplify → *Working Model*: Identify and select factors to describe important aspects of *Real World Problem*; determine those factors that can be neglected.



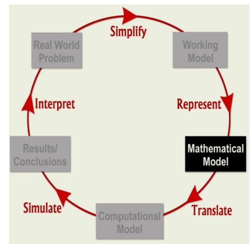
- State simplifying assumptions.
- Determine governing principles, physical laws.
- Identify model variables and inter-relationships.

Example: Falling Rock

- Governing principles: **d = v*t** and **v = a*t**.
- Simplifying assumptions:
  - Gravity is the only force acting on the body.
  - Flat earth.
  - No drag (air resistance).
  - Model variables are H,V, g; t, x, and v
  - Rock's position and velocity above the ground will be modeled at discrete times (t0, t1, t2, …) until rock hits the ground.

Mathematical Model

Represent → Mathematical Model: Express the *Working Model* in mathematical terms; write down mathematical equations whose solution describes the *Working Model.*



In general, the success of a mathematical model depends on how easy it is to use and how accurately it predicts.

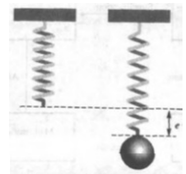
Typical Relation Between Variables

- Proportionality
- Two Variables x and y are proportional (to each other) of one is always a constant multiple of the order: x=c*y or x/y=c

We now discuss an example from the reference textbook, the spring and mass system. This will be only "traditional" example that will be discussed in this course. We will use instead, more intuitive examples from image analysis (and other related ones that use some important techniques of machine learning).

Spring Mass

- Find the relation between the elongation of the spring and the mass attached to it (see the figure on the right)
- Real World Data: (mass, elongation)
  (50,1.000), (100,1.875), (150,2.750), …
- Visualization:
  plot these points
- Name the Variables: m – mass, e – elongation
- Simplification: e is proportional to m, e=c*m
- Modeling: find (estimate) the constant c
- Interpretation and verification: plot and see if the line is "close" to the points



Spring–mass system

Mass	Elong
50	1.000
100	1.875
150	2.750
200	3.250
250	4.375
300	4.875
350	5.675
400	6.500
450	7.250
500	8.000
550	8.750

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Example: Falling Rock

v0	v1	v2	…	vn
x0	x1	x2	…	xn
t0	t1	t2	…	tn

t0 = 0; x0 = H; v0 = V

$t1 = t0 + \Delta t$ $\qquad$ $t2 = t1 + \Delta t$

$x1 = x0 + (v0 * \Delta t)$ $\qquad$ $x2 = x1 + (v1 * \Delta t)$

$v1 = v0 - (g * \Delta t)$ $\qquad$ $v2 = v1 - (g * \Delta t)$

…

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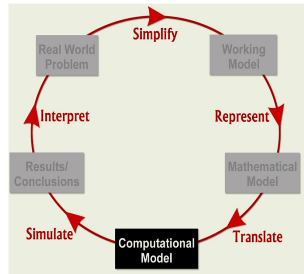
Computational Model

Translate → Computational Model:



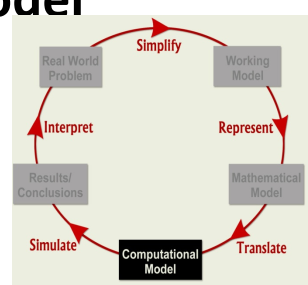
Change *Model* into a form suitable

for computational solution.

- Existence of unique solution
- Choice of the numerical method
- Choice of the algorithm
- Software

Computational Model

Translate → Computational Model: Change *Mathematical Model* into a form suitable for computational



Computational models include software such as Maple, Matlab, Maple, Excel, or Mathematica, or languages such as Fortran, C, C++, or Java.

Example: Falling Rock

Pseudo Code

Input

V, initial velocity; **H**, initial height

g, acceleration due to gravity

Δt, time step; **imax**, maximum number of steps

Output

ti, t-value at time step i

xi, height at time ti

vi, velocity at time ti

Example: Falling Rock

Initialize

Set ti = t0 = 0; vi = v0 = V; xi = x0 = H

print ti, xi, vi

Time stepping: i = 1, imax

Set ti = ti + Δt

Set xi = xi + vi*Δt

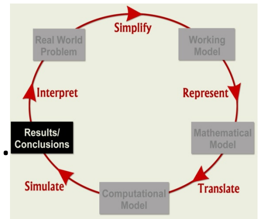
Set vi = vi - g*Δt

print ti, xi, vi

if (xi <= 0), Set xi = 0; quit

Results/Conclusions

Simulate → *Results/Conclusions*:
Run "Computational Model"
to obtain *Results*; draw *Conclusions*.



- Verify your computer program; use check cases; explore ranges of validity.
- Graphs, charts, and other visualization tools are useful in summarizing results and drawing conclusions.

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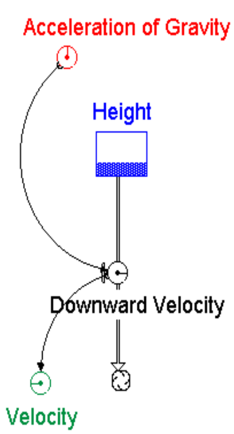
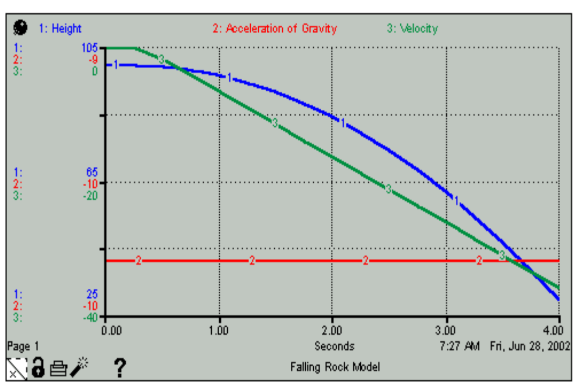
Falling Rock: Model





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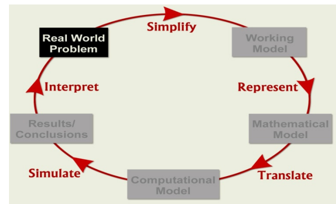
Real World Problem

Interpret *Conclusions:*

Compare with *Real World Problem* behavior.

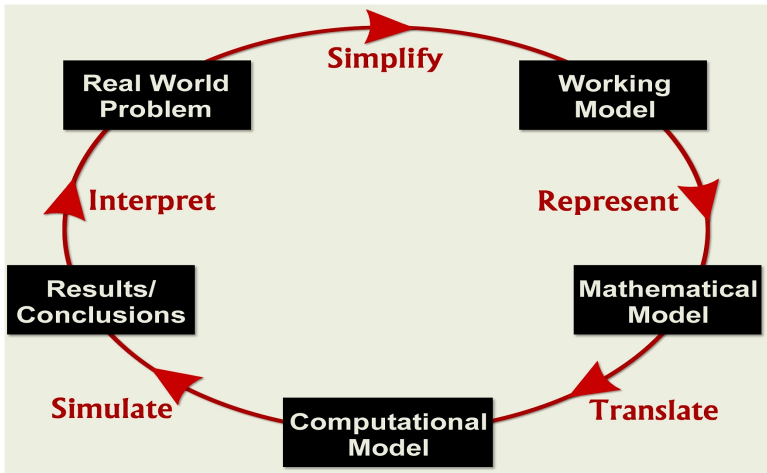


- If model results do not "agree" with physical reality or experimental data, reexamine the Working Model (relax assumptions) and repeat modeling steps.
- Often, the modeling process proceeds through several iterations until model is "acceptable".

Example: Falling Rock

- To create a more realistic model of a falling rock, some of the simplifying assumptions could be dropped; e.g., incor-porate drag - depends on shape of the rock, is proportional to velocity.
- Improve discrete model:
  - Approximate velocities in the midpoint of time intervals instead of the beginning.
  - Reduce the size of Δt.

Mathematical Modeling Process



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Structure of the course

- Principles of modeling (file: introduction-principles.ppt)
- Basic numerical methods:
  - Root finding
  - Interpolation
  - Least square methods
  - Numerical quadratures
  - ODE’s
  - PDE’s

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Reference

- Maple, Matlab, …
- Chapra & Canale: Numerical Methods for Engineers
- Klamkin: Mathematical Modeling