In Service of Dreams - The Science and Practice of Water Quality Modeling

Robert B. Ambrose, Jr.

November, 2013

1. Dreams and Goals

Where there is no vision, the people perish

… your young men shall see visions,
and your old men shall dream dreams

You may say that I'm a dreamer
but I'm not the only one…

Dreams Elevate Thought
they define humanity

… And I have felt
A presence that disturbs me with the joy
Of elevated thoughts; a sense sublime
Of something far more deeply interfused,
Whose dwelling is the light of setting suns,
And the round ocean, and the living air,
And the blue sky, …

Therefore am I still
A lover of the meadows and the woods,
And mountains; and of all that we behold
From this green earth; …

From "Lines Written a Few Miles Above Tintern Abbey, on Revisiting the Banks of the Wye during a Tour, July 13, 1798," by William Wordsworth

Dreams Sustain the Weary

through the joyless slog
and the interminable meeting

But oft, in lonely rooms, and mid the din
Of towns and cities, I have owed to them,
In hours of weariness, sensations sweet, …

In darkness, and amid the many shapes
Of joyless daylight; when the fretful stir
Unprofitable, and the fever of the world,
Have hung upon the beatings of my heart,
How oft, in spirit, have I turned to thee
O sylvan Wye!

From "Lines Written a Few Miles Above Tintern Abbey, on Revisiting the Banks of the Wye during a Tour, July 13, 1798," by William Wordsworth

Dreams of Gaia

Dreams of Science

Carl Sagan
astronomy, cosmology

Eugene Odum
ecology

The Consequence of Dreams

They kick off a chain of causation

Dreams → Goals → Action → Results

The Consequence of Dreams

In the water quality realm

Dreams

Robust environment
Healthy population

Goals

Fishable, swimmable waters
WQ standards and criteria

Action

TMDL, WLA programs
WWTP construction,
Buffer strips

Results

Less enrichment, TSS, bacteria
More DO, clarity, fish

The Consequence of Dreams

with bottom-up feedback

The National Reaction to a Dream

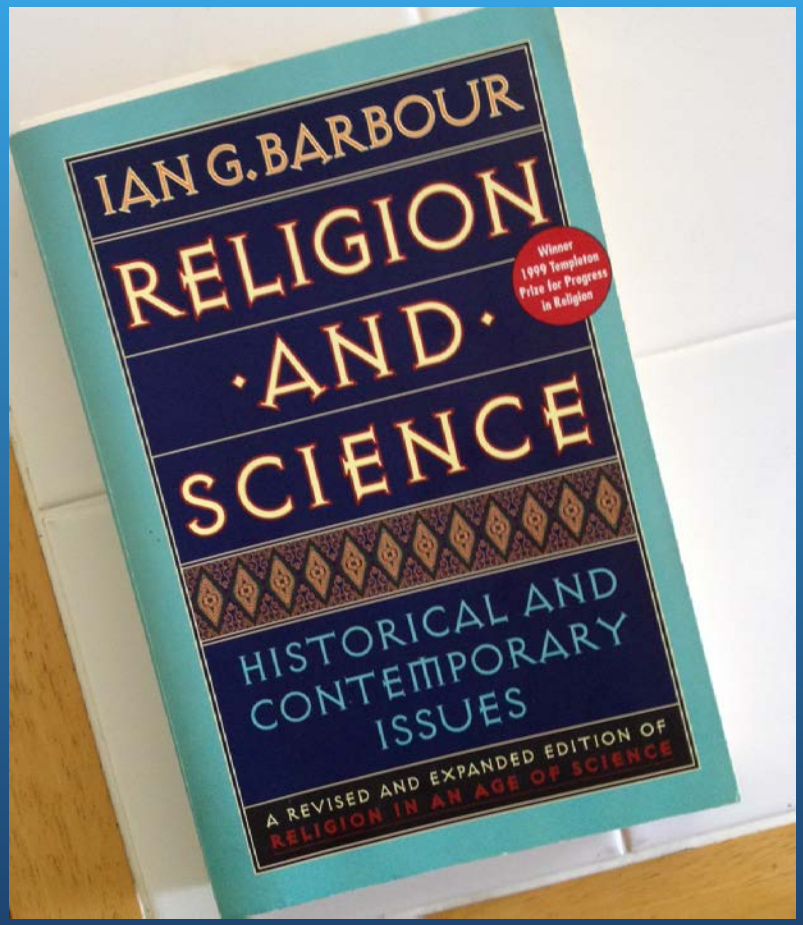
To save the earth

- The image of Gaia, December 1968
- Earth Day, April 1970
- Founding of EPA, December 2, 1970
  - Protect human health and the environment
- Legislation to protect water (selections)
  - Water Pollution Control Act, 1948
  - Clean Waters Restoration Act, 1966
  - Water Quality Improvement Act, 1970
  - Federal Water Pollution Control Amendments of 1972
  - Clean Water Act, 1977
  - Water Quality Act, 1987

Clean Water Act

- "It is a national goal that the discharge of pollutants into the navigable waters be eliminated by 1985."
- TMDL focused on protection of surface water resources
  - Streams
  - Reservoirs
  - Estuaries
- The ultimate goal of the TMDL process is to meet the water quality standards and ultimately improve habitat in a watershed.

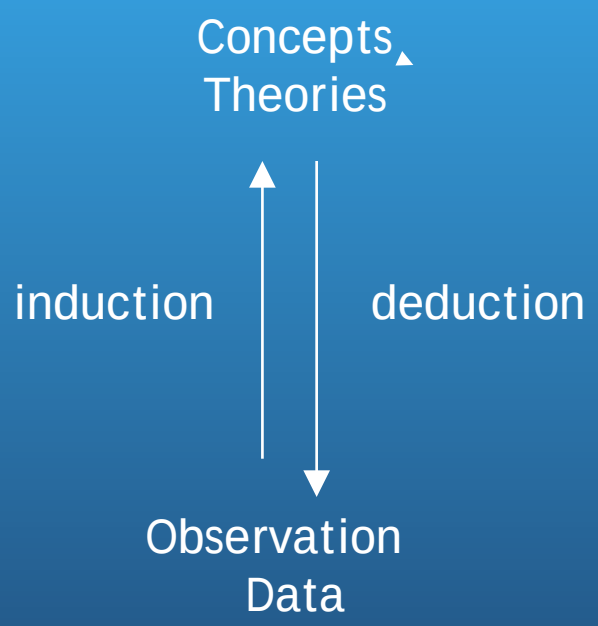
2. Science and Truth



From Barbour, I. “Religion and Science – Historical and Contemporary Issues” HarperCollins, 1997.

The Structure of Science

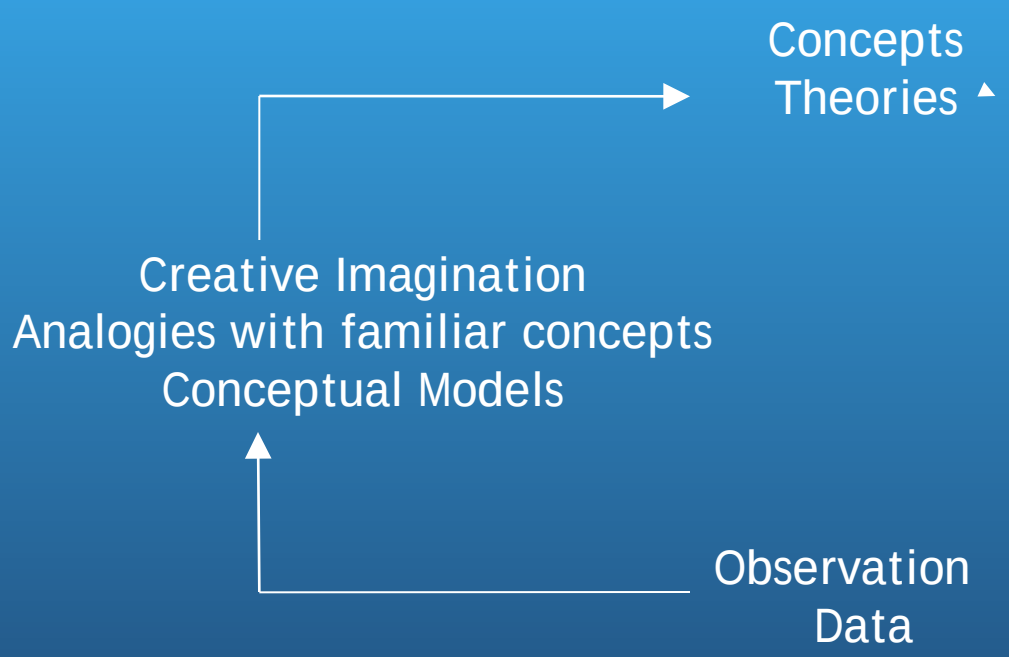
Traditional View:



From Barbour, I. “Religion and Science – Historical and Contemporary Issues” HarperCollins, 1997.

The Structure of Science

Modified View of Induction:

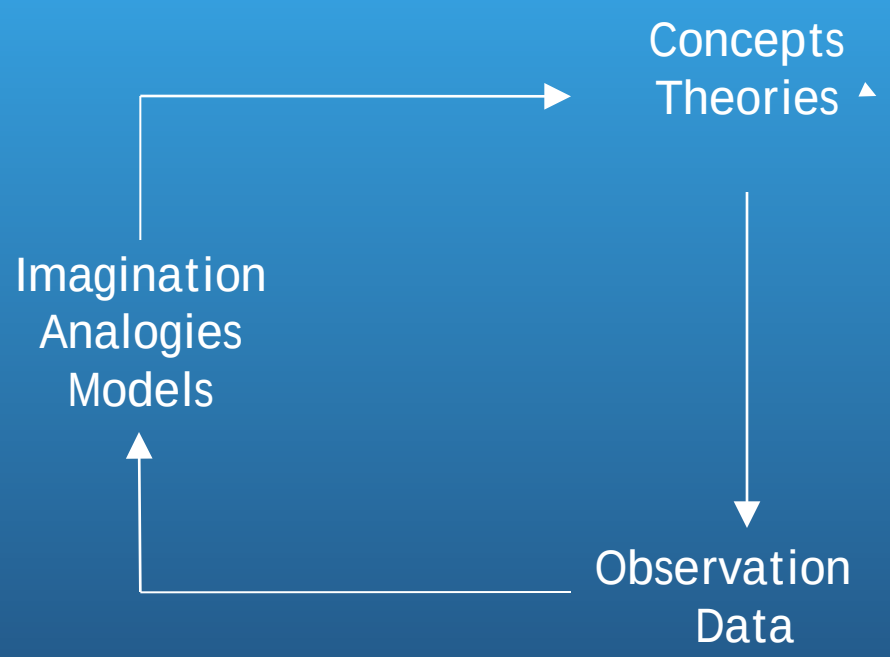


Theories involve novel concepts not found in the data, so no direct path from data to theory.

From Barbour, I. “Religion and Science – Historical and Contemporary Issues” HarperCollins, 1997.

The Structure of Science

Hypothetico-deductive approach:



A valid theory leads to expected observations.

Objective data can be used to falsify (never verify) theory.

(Karl Popper)

From Barbour, I. "Religion and Science – Historical and Contemporary Issues" HarperCollins, 1997.

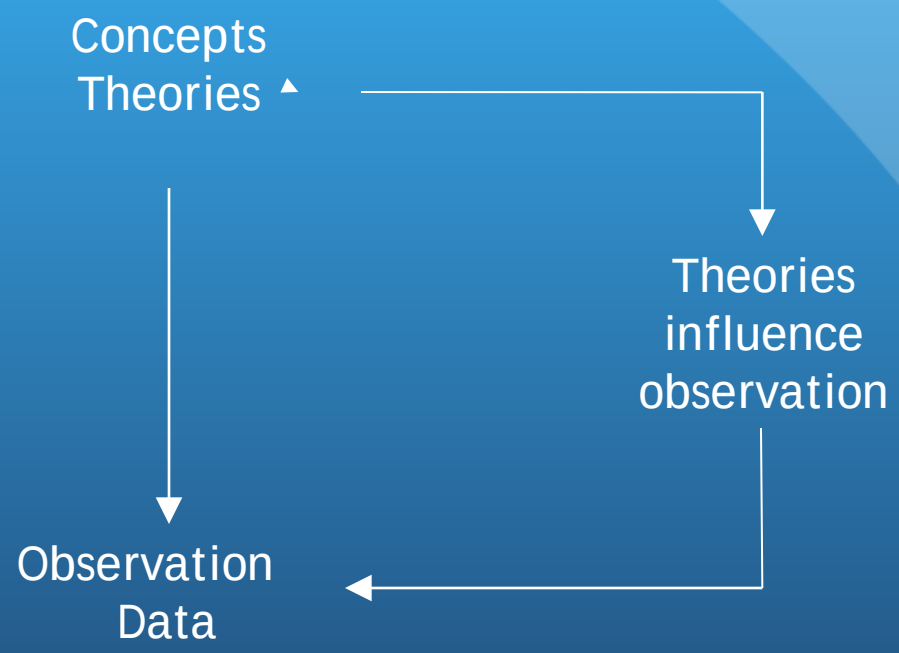
The Structure of Science

Problems with hypothetico-deductive approach:

A theory cannot be tested alone, but only within a network of theories and auxiliary hypotheses.

All data are theory-laden.

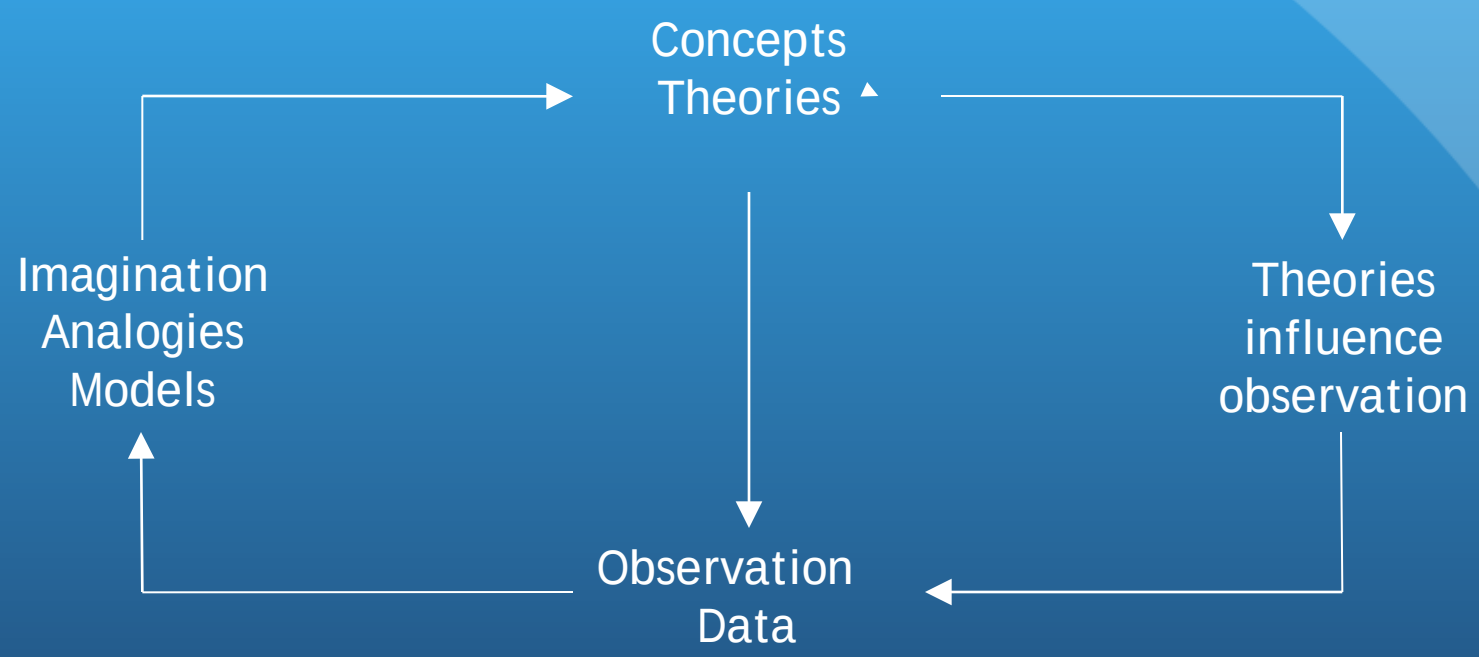
Observation can alter object.



From Barbour, I. "Religion and Science – Historical and Contemporary Issues" HarperCollins, 1997.

The Structure of Science

Paradigms, a cluster of concepts and data (Thomas Kuhn):



From Barbour, I. “Religion and Science – Historical and Contemporary Issues” HarperCollins, 1997.

So what is truth?

Three views:

- Correspondence view
  - Proposition true if it corresponds to reality
- Coherence view
  - Proposition true if comprehensive and internally coherent
- Pragmatic view
  - Proposition true if it works in practice

From Barbour, I. “Religion and Science – Historical and Contemporary Issues” HarperCollins, 1997.

So what is truth?

Three views:

The *meaning* of truth

- **Correspondence view**
  - **Proposition true if it <u>corresponds to reality</u>**

But reality is inaccessible to us

- Coherence view
  - Proposition true if comprehensive and internally coherent

- Pragmatic view
  - Proposition true if it works in practice

From Barbour, I. "Religion and Science – Historical and Contemporary Issues" HarperCollins, 1997.

How do we determine truth?

Criteria for assessing theories:

- Agreement with data
- Coherence
- Scope
- Fertility

From Barbour, I. “Religion and Science – Historical and Contemporary Issues” HarperCollins, 1997.

How do we determine truth?

Criteria for assessing theories:

- Agreement with data
  - Most important criterion, but
  - Never proves a theory true
  - Other theories may fit data
  - Theories are always underdetermined by data
  - Disagreement with data does not prove theory false
  - Predictive success is strong support for theory
- Coherence
- Scope
- Fertility

From Barbour, I. “Religion and Science – Historical and Contemporary Issues” HarperCollins, 1997.

How do we determine truth?

Criteria for assessing theories:

- Agreement with data
- Coherence
  - Internal coherence and simplicity, elegance
  - Conceptual consistency with other theories
- Scope
- Fertility

From Barbour, I. “Religion and Science – Historical and Contemporary Issues” HarperCollins, 1997.

How do we determine truth?

Criteria for assessing theories:

- Agreement with data
- Coherence
- Scope
  - Comprehensiveness and generality
  - Unification of disparate domains
  - Supported by a variety of evidence
- Fertility

From Barbour, I. “Religion and Science – Historical and Contemporary Issues” HarperCollins, 1997.

How do we determine truth?

Criteria for assessing theories:

- Agreement with data
- Coherence
- Scope
- Fertility
  - Providing framework for ongoing research
  - Fruitful in generating hypotheses and experiments

From Barbour, I. “Religion and Science – Historical and Contemporary Issues” HarperCollins, 1997.

In Summary, *Critical Realism*

- Science does not lead to certainty.
- Conclusions are always incomplete, tentative, subject to revision.
- Theories change in time.
- But science offers reliable procedures for testing and evaluating theories.

From Barbour, I. "Religion and Science – Historical and Contemporary Issues" HarperCollins, 1997.

3. Building Simulation Models

in support of environmental regulation

Models Serve as a Bridge Between Science and Regulation

Environmental Science

Environmental Regulation

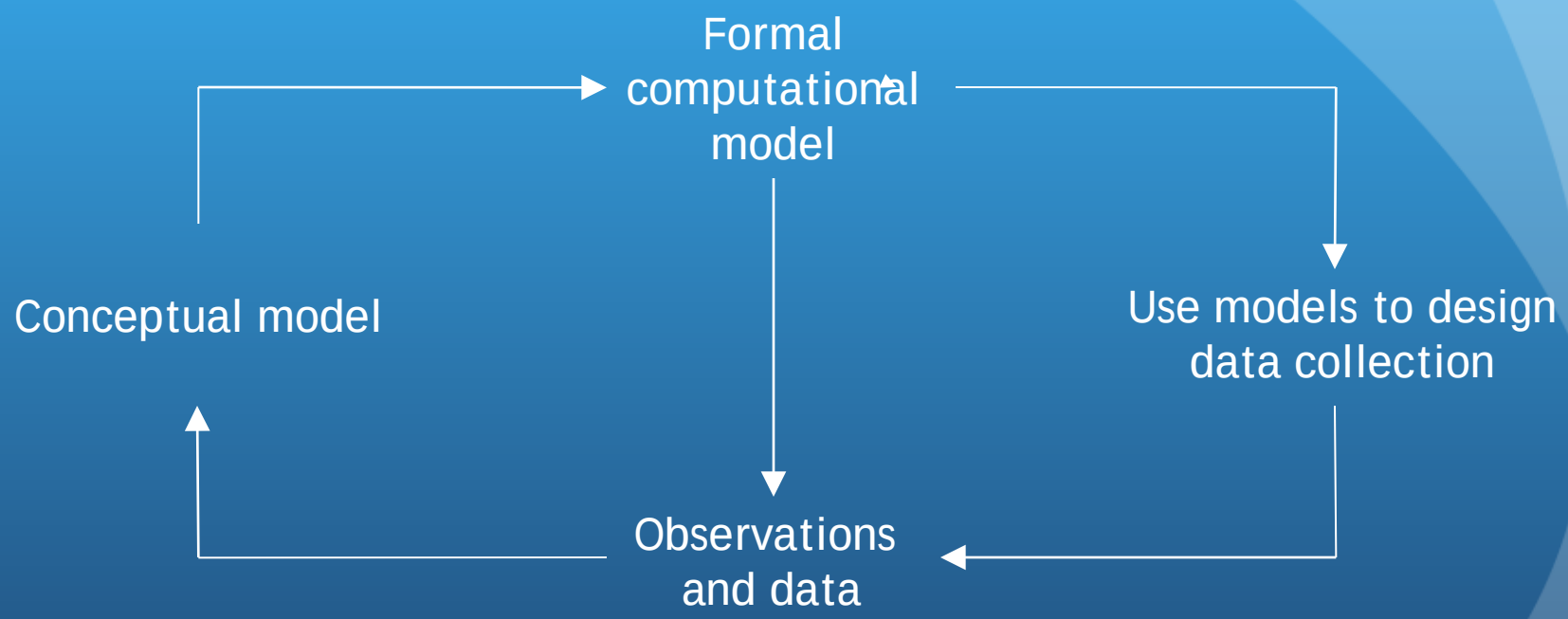
User Constructs Particular Models

for specific water bodies and regulations

- General purpose modeling programs such as WASP*, QUAL2*, CE-QUAL-*, are not “models” *per se*

- General purpose program becomes a water body model when the user supplies input data
  - Computational network
  - Constants and Parameters
  - Environmental forcing functions

Development of Computational Models

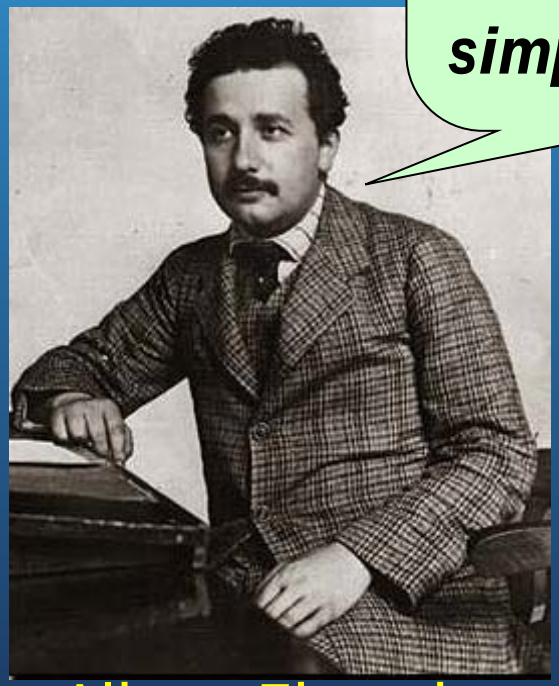


Two General Approaches

- Start with simple model
  - Build complexity as necessary
- Start with comprehensive model
  - Test and remove elements found unnecessary

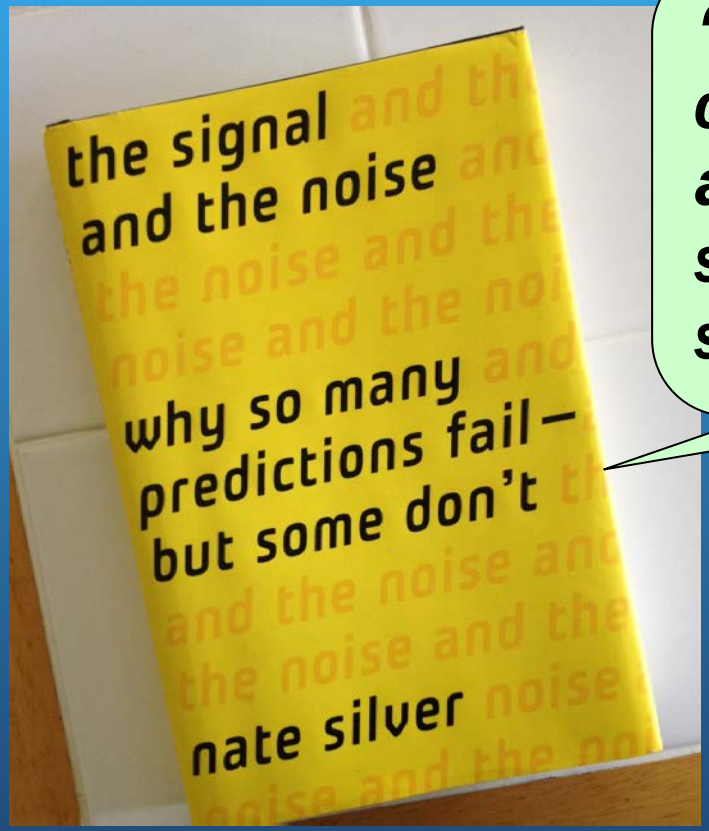
Goal of Model Complexity

"Make things as simple as possible, but not any simpler."



Albert Einstein

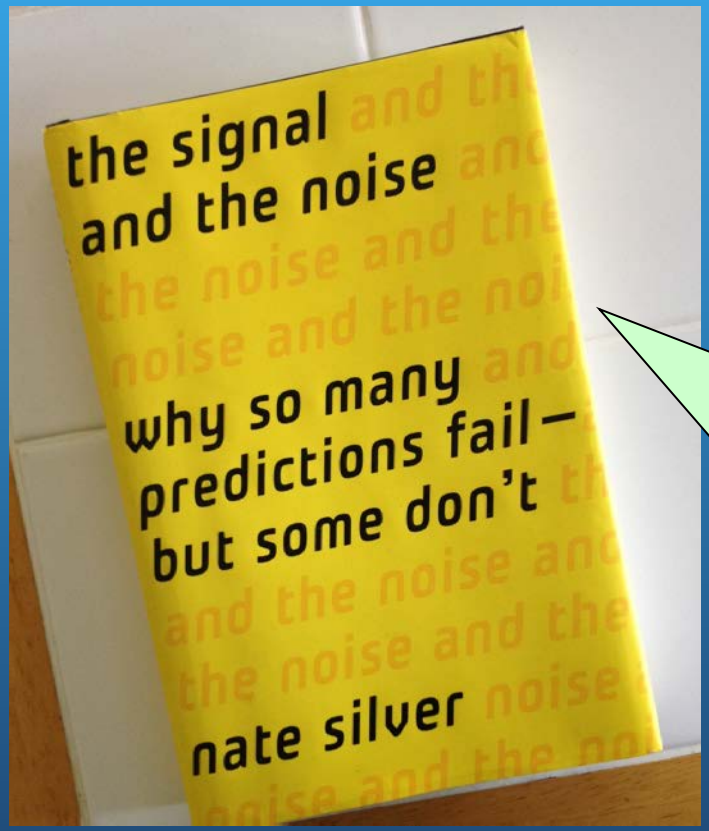
Goal of Model Complexity



"While simplicity can be a virtue… a model should be sophistically simple."

From Silver, Nate. "The Signal and the Noise ," The Penguin Press, N.Y., 2012.

Goal of Model Complexity



"The goal of any predictive model is to capture as much signal as possible and as little noise as possible."

From Silver, Nate. "The Signal and the Noise ," The Penguin Press, N.Y., 2012.

The Silver Path to Better Prediction

- **Believe in objective truth and commit to pursue it**
- Realize that we perceive truth imperfectly
  - Many theories (models), when tested, give poor results
  - Many untested theories (models) are wrong
  - We may be living with delusion
- Be appropriately cautious
  - All models wrong, but some useful (George Box)
  - Strange results are usually “bug” not “eureka”
  - Good models can be useful even when they fail
    - Understand how they are wrong
    - Know what to do next

From Silver, Nate. “The Signal and the Noise ,” The Penguin Press, N.Y., 2012.

The Silver Path to Better Prediction

- Believe in objective truth and commit to pursue it
- **Realize that we perceive truth imperfectly**
  - **Many theories (models), when tested, give poor results**
  - **Many untested theories (models) are wrong**
  - **We may be living with delusion**
- Be appropriately cautious
  - All models wrong, but some useful (George Box)
  - Strange results are usually “bug” not “eureka”
  - Good models can be useful even when they fail
    - Understand how they are wrong
    - Know what to do next

From Silver, Nate. “The Signal and the Noise ,” The Penguin Press, N.Y., 2012.

The Silver Path to Better Prediction

- Believe in objective truth and commit to pursue it
- Realize that we perceive truth imperfectly
  - Many theories (models), when tested, give poor results
  - Many untested theories (models) are wrong
  - We may be living with delusion
- Be appropriately cautious
  - All models wrong, but some useful (George Box)
  - Strange results are usually “bug” not “eureka”
  - Good models can be useful even when they fail
    - Understand how they are wrong
    - Know what to do next

From Silver, Nate. “The Signal and the Noise ,” The Penguin Press, N.Y., 2012.

Balanced Model Complexity

When building a water body model, adjust complexity to match the problem:

- More Complex ***Aquatic Systems***
- More Complex ***Water Quality Processes***
- More Complex ***Management Questions***

Complexity of Aquatic Systems

- Simplest
  - Ponds and shallow reservoirs
  - Controlled streams and rivers
- Intermediate
  - Watersheds and river basins
  - Well mixed estuaries
  - Small lakes and reservoirs
- Most Complex
  - Wetlands
  - Stratified estuaries and coastal waters
  - Large lakes and reservoirs

Complexity of Water Quality Processes

- Simplest
  - Salinity, conservative tracers
  - Simple toxicants
  - Dissolved oxygen-CBOD (effluent dominated)
- Intermediate
  - pH – alkalinity
  - Non-ionic toxicants, cationic metals
  - Dissolved oxygen-CBOD-nutrient enrichment
- Most Complex
  - Sediment transport
  - Anionic metals, such as mercury
  - Phytoplankton – benthic algae – macrophyte

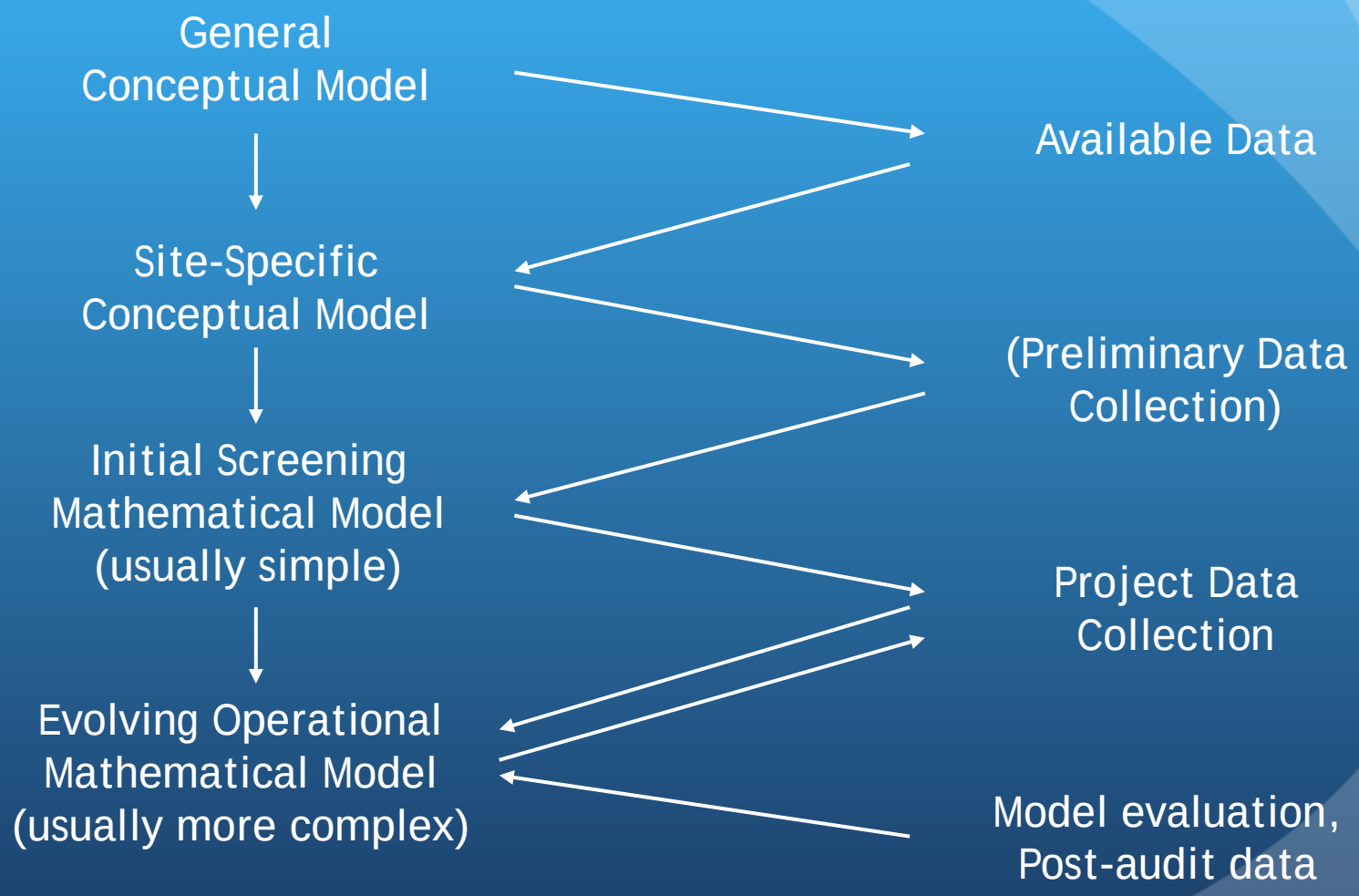
More Complex Management Questions

- the ***spatial and temporal distributions*** of target pollutants under various management scenarios
- the relative ***contributions of various sources*** of pollutants over time
- the likely ***pollutant attenuation trajectories*** and times to recovery under various management scenarios
- the relative effects of ***transient or extreme events***, such as spills or storms
- the possible effects of ***poorly understood*** environmental events

General Constraints in Applied Regulatory Modeling

- Time
- Resources
- Regulatory language
- Scientific credibility

Iterative Model Development Process



How Complex Should Final Computational Model Be?

Final model balances:

- The complexity of the environmental system.
- The complexity of the water quality processes.
- The management questions and related need for accuracy.

How Complex Should Final Computational Model Be?

Consequences for overly simple models:

- Miss key processes and extrapolate inaccurately.
- May not address relevant management questions.
- May not be defensible to adversarial review.
- Insufficiently adaptable to changing management requirements.

How Complex Should Final Computational Model Be?

Consequences for overly complex models:

- Adds unnecessary data collection and computational burdens.
- Adds to uncertainty.
- Causes overconfidence, leads astray. (Silver)
- Shifts focus away from problem solutions to endless analysis.

General Approach: Combine monitoring and modeling

Monitoring

- Characterizes the site
- Characterizes pollutant distribution in space and time
- Characterizes important environmental conditions

Modeling

General Approach: Combine monitoring and modeling

Monitoring

Modeling

- Integrates general process knowledge with site specific data
- Enforces mass balance consistency
- Provides framework to extend the data
  - Sensitivity analysis, hindcast, forecast, scenario evaluation

4. Components of Water Quality Models

Physical Component - Traditional

- Surface water
- Benthic sediment
- Flood plain
- Riparian wetlands
- Watershed
- Ground water
- Atmosphere

Model

Boundary fluxes or multipliers

Physical Components - Modern

- Surface water network
- Benthic sediment

Toxicant models; SOD modules

- Flood plain
- Riparian wetlands
- Watershed surface
- Ground water
- Atmosphere

External models, modules, functions

Physical Components - Watershed

- Surface water network
- Benthic sediment
- Flood plain
- Riparian wetlands
- Watershed surface
- Ground water
- Atmosphere

Watershed models

Boundary fluxes or multipliers

Physical Components - Multimedia

- Surface water
- Benthic sediment
- Flood plain
- Riparian wetlands
- Watershed surface
- Ground water
- Atmosphere

Linked models, modules, functions

Process Components - Traditional

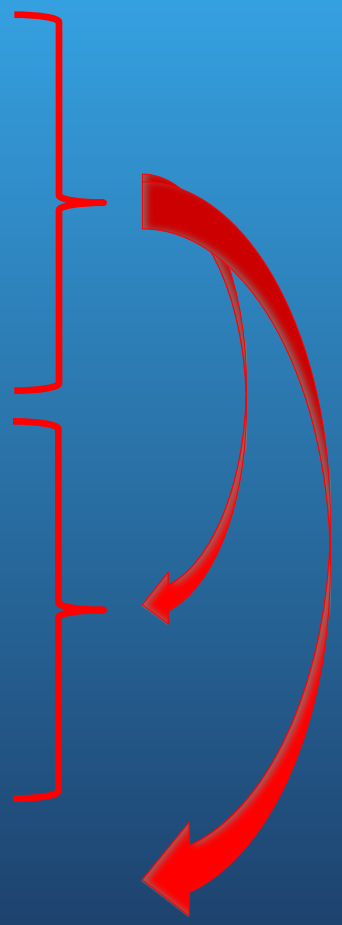
- Hydrodynamics
- Water transport
- Heat balance
- Sediment transport
- Dissolved oxygen balance
- Nutrient cycling
- Algal dynamics
- pH – alkalinity
- Pollutant degradation

Process Components – Advanced Riverine

- Hydrodynamics
- Water transport
- Heat balance
- Sediment transport
- Dissolved oxygen balance
- Nutrient cycling
- Algal dynamics
- pH – alkalinity
- Pollutant degradation

Process Components – Advanced Hydrodynamics

- Hydrodynamics
- Water transport
- Heat balance
- Sediment transport
- Dissolved oxygen balance
- Nutrient cycling
- Algal dynamics
- pH – alkalinity
- Pollutant degradation



Watershed Modeling Tools

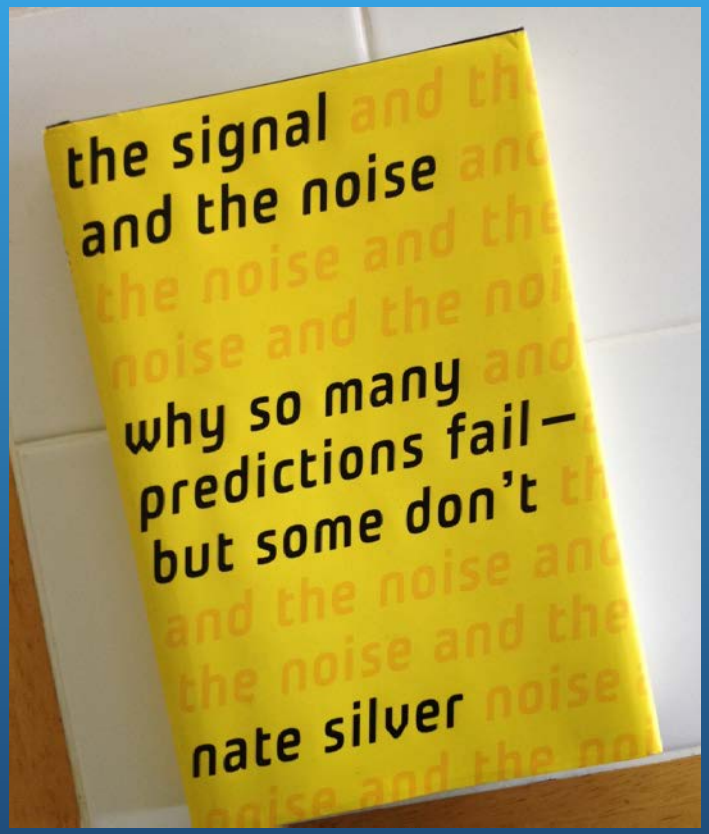
- Data and Databases
- Mapping and GIS Frameworks
- Assessment Tools
- Simulation Models

General Modeling Approaches

- Loose integration –
  - “toolkit approach”
- Tight integration –
  - “mega-modeling approach”

5. Uncertainty and Forecasting

Some general observations adapted from Silver



From Silver, Nate. "The Signal and the Noise ," The Penguin Press, N.Y., 2012.

The Importance of Computer Analysis to Forecasting Depends

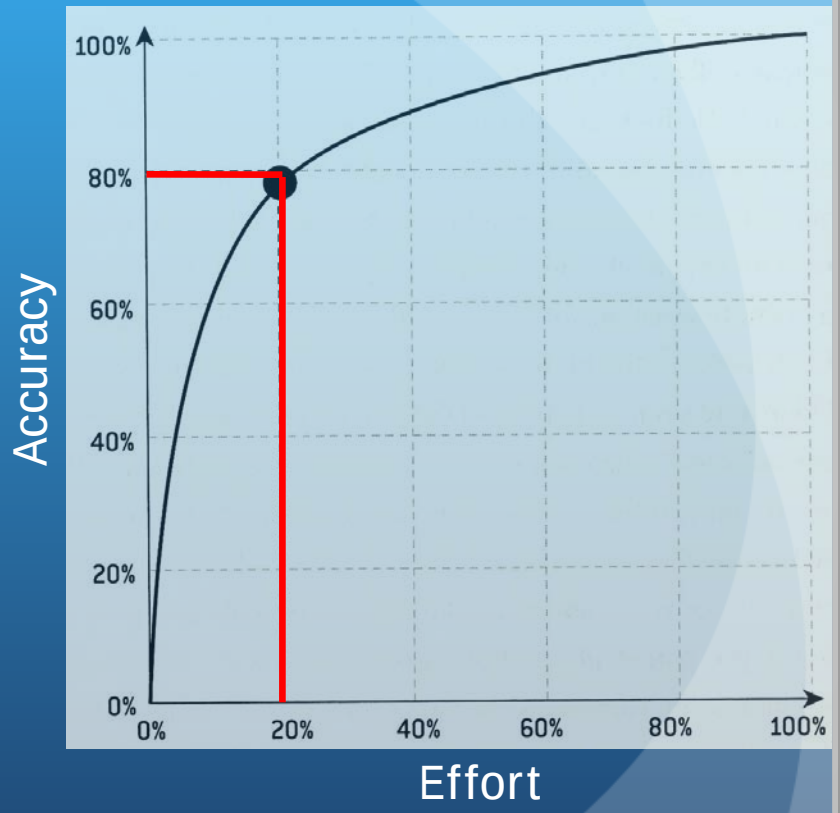
- Most useful when
  - System abides by relatively simple laws
  - These laws are well understood
- Less useful when
  - Understanding root causes are blurrier
  - The observational data are noisier

From Silver, Nate. “The Signal and the Noise ,” The Penguin Press, N.Y., 2012.

Pareto Principle of Prediction:

Getting a few things right can go a long way.

- Right data
  - More better than less
  - Quality controlled
- Right technology
  - Top-shelf tools nice
  - Know how to use what you have
- Right incentive
  - Care about accuracy

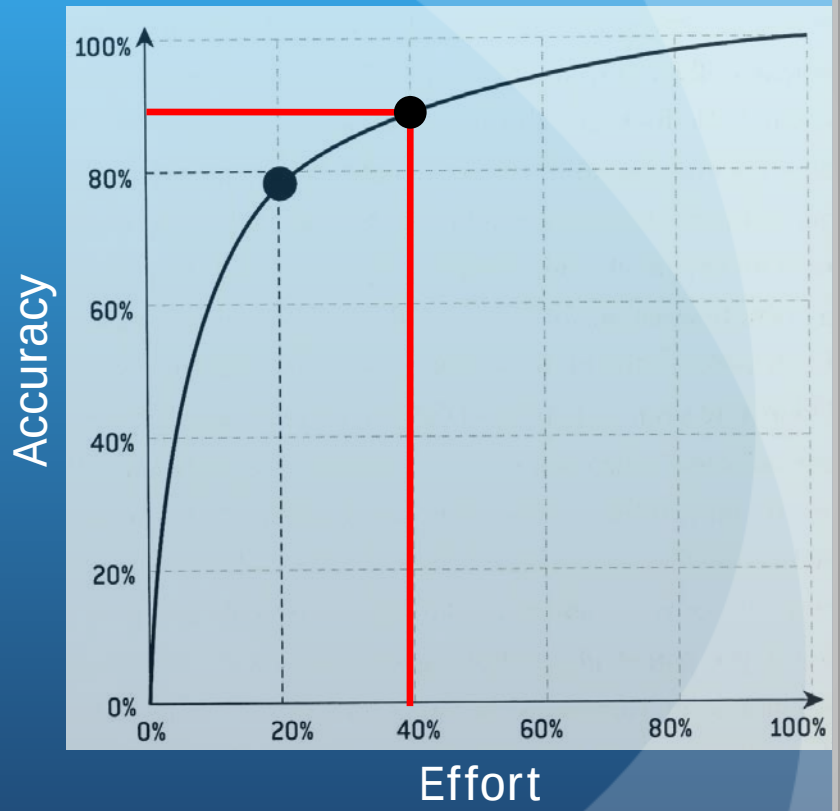


From Silver, Nate. “The Signal and the Noise ,” The Penguin Press, N.Y., 2012.

Intermediate Steps in Prediction:

Modest steps lead to reasonable improvements

- Develop experience, apply common sense
- Master rules of thumb (heuristics)
- Beyond *ad hoc* application to systematic process

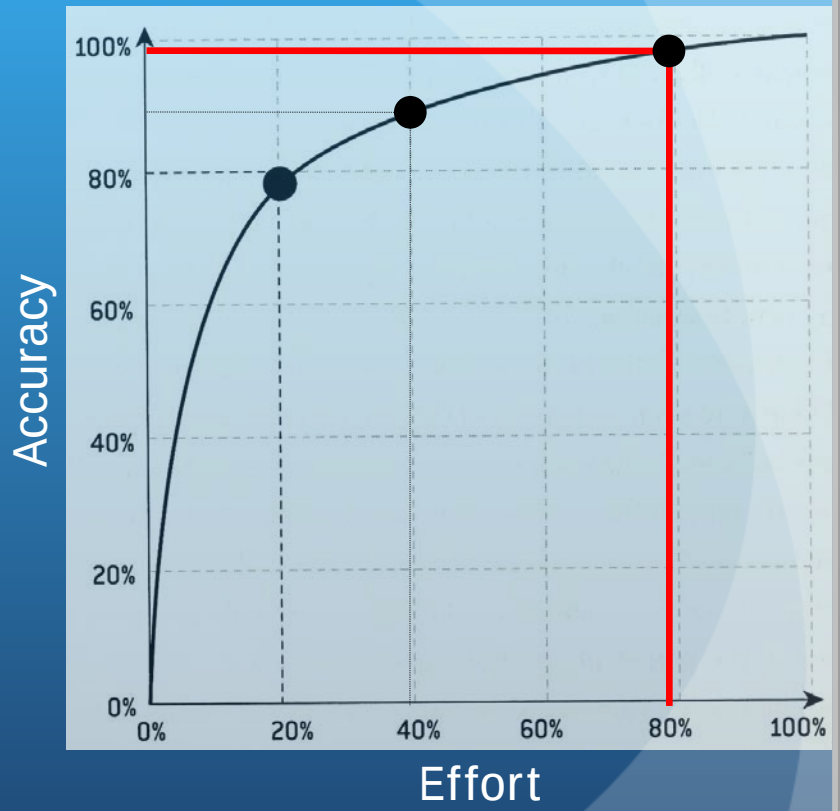


From Silver, Nate. “The Signal and the Noise ,” The Penguin Press, N.Y., 2012.

Expert Level Prediction:

Much more effort, diminishing returns … but may be required in adversarial situations

- Thoroughly master theory
- Apply more variables and complexity
- Learn exceptions to rules of thumb
- Apply more subtle strategies



From Silver, Nate. “The Signal and the Noise ,” The Penguin Press, N.Y., 2012.

Know Your Sources of Uncertainty

- Initial conditions
- Boundary conditions
- Environmental forcing functions
- Temporal variability
- Spatial variability
- Structural uncertainty in the model
- Scenario uncertainty

Forecasting as a Bayesian

- Know where you're coming from (The Prior)
  - Conventional theory
  - Applied models with literature data
  - Common sense
- Try, and err
  - Update forecasts as new data become available
  - Appreciate the amount of noise in the data
  - Be wary of the bias weighting the last data point
  - Be willing to change when facts change

From Silver, Nate. "The Signal and the Noise ," The Penguin Press, N.Y., 2012.

Draw on Scientific Knowledge and Self Knowledge – The Modeler's Serenity Prayer

- The serenity to accept things we cannot predict
- The courage to predict the things we can
- The wisdom to know the difference

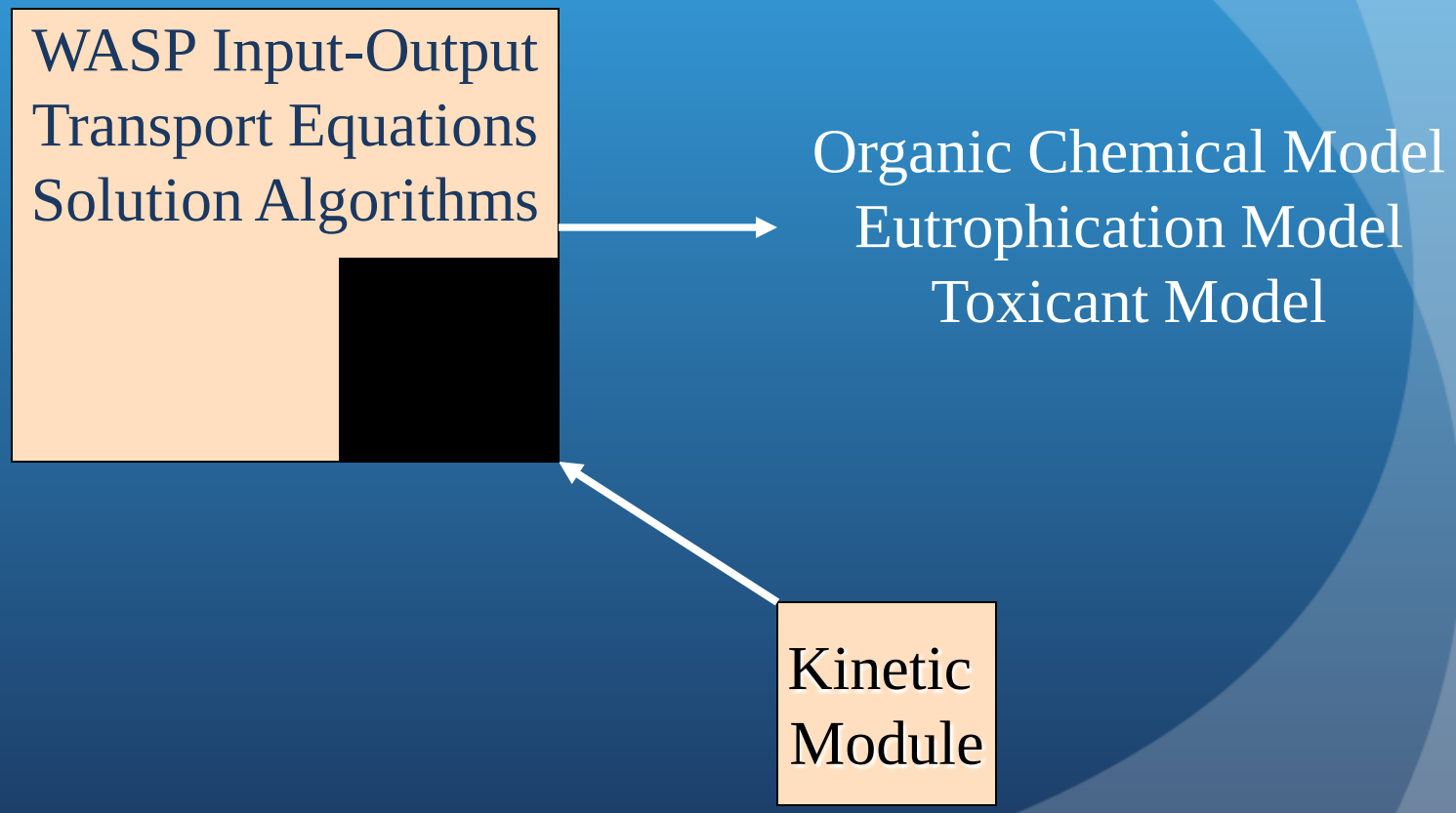
From Silver, Nate. "The Signal and the Noise ," The Penguin Press, N.Y., 2012.

6. Dreams, Revisited

My personal version

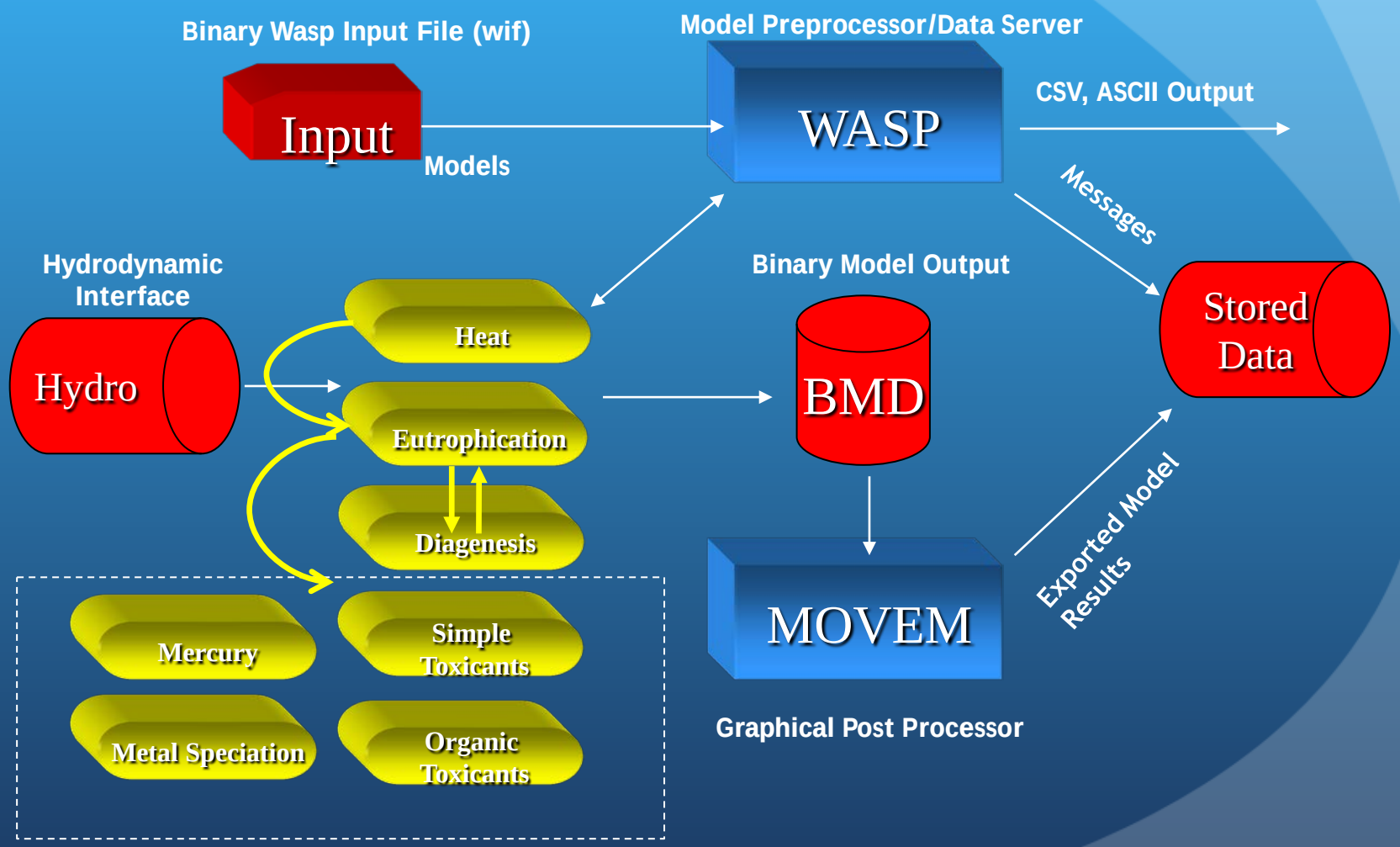
Dreams of a Modeling Community

Origins – early WASP model structure:



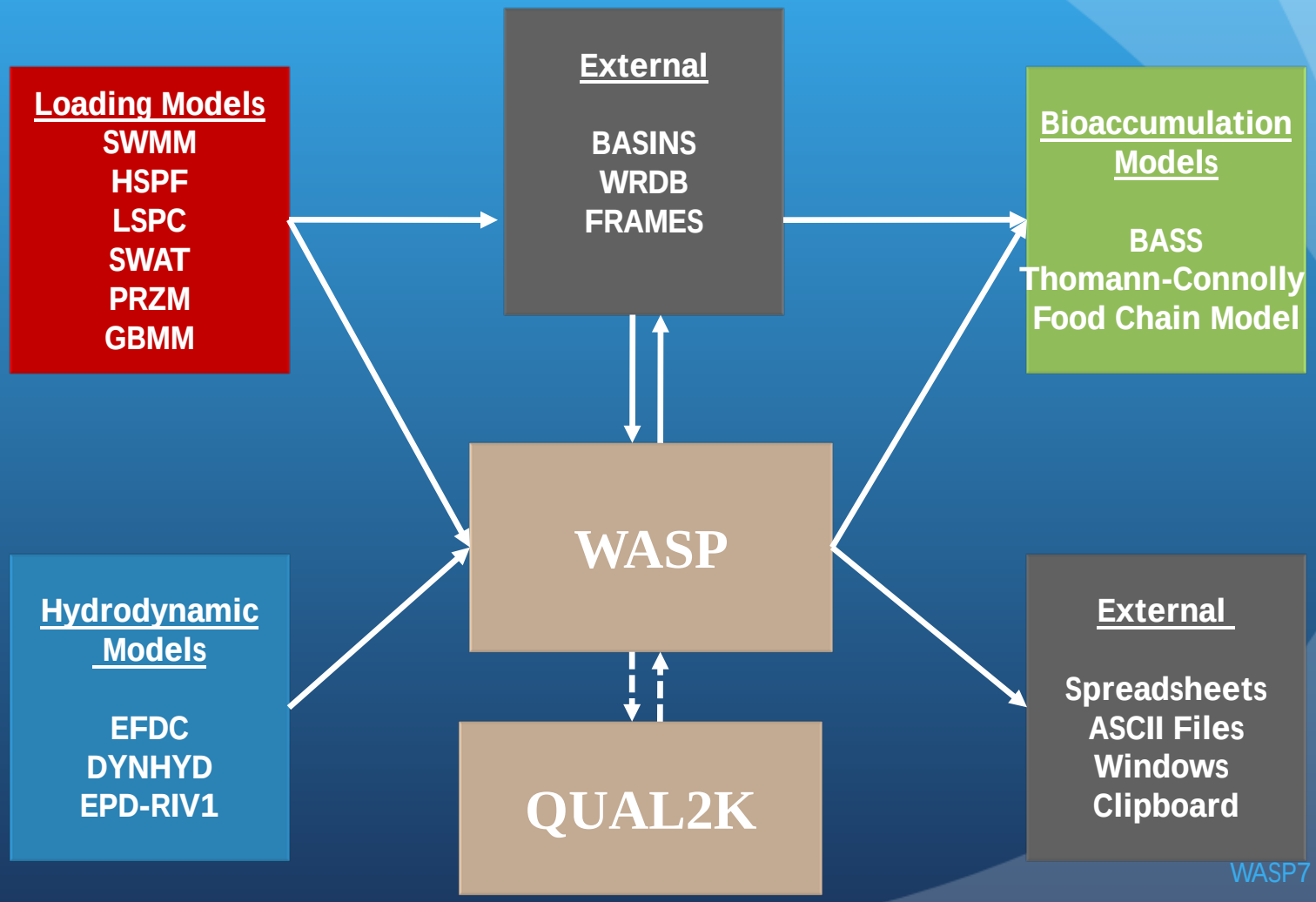
Dreams of a Modeling Community

Development of WASP infrastructure



Dreams of a Modeling Community

Development of WASP external linkages

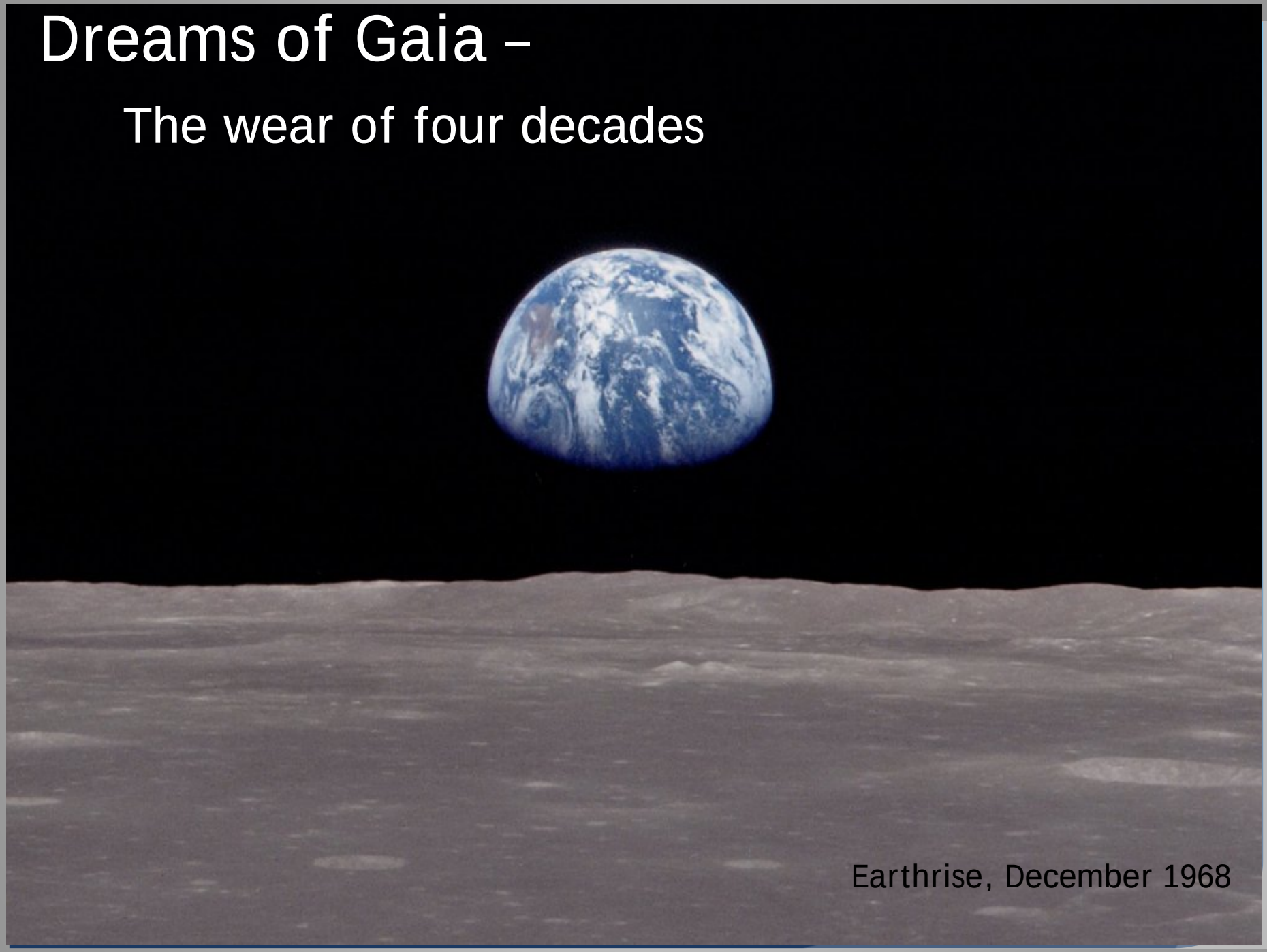


Dreams of a Modeling Community

- Adoption of standard linkage protocols
  - Hydrodynamics and sediment transport
  - Watershed loading
- Development of generic modules as general dll's
  - Modeling utilities
    - Graphics
    - Statistics
  - Water quality submodules
    - Sediment diagenesis
    - Pollutant fate (e.g., PCB's, mercury)
    - Algal dynamics (e.g., phytoplankton, periphyton classes

Dreams of Gaia –

The wear of four decades



A Dream in China Yangtze Blues

Highlands of Hubei, Three Gorges

Far away, well east of Eden
virile rivers carved a valley
through the age of long ago.

...

Reflections in Poetry, at bobambrosejr-poetry.blogspot.com

A Dream in China

Yangtze Blues

Here in the highlands of Hubei
I can hear its song
rising out of mist and mountain
gray home of gods now gone
refuge of wayfaring mystic and misfit
place where the wild torrent
courses through gorges
once upon some time ago.

A Dream in China

Yangtze Blues

But now the long river
languishes
flat and heavy
murky deepness drowns Three Gorges
sighs behind a concrete slab
controlled and still
until release.

A Dream in China

Yangtze Blues

A brand new land
of grit and coal
of dusky skies
that smother cities

town and village
torn and pillaged
taken into concrete

borg ...

... soar

into the gray-brown
skyscape, lined
with cranes

and belching stacks
that stitch the land

and sky with smog
and seal the earth

beneath the load
of human progress

East meets West
and ups the ante

heeds the siren
staggers forward

fading into midday haze.

Photograph from posting in io9.com, 4/02/13, by Robert T. Gonzalez

Reflections in Poetry, at bobambrosejr-poetry.blogspot.com

A Dream in China

Yangtze Blues

And from the highlands of Hubei
so very far away from Eden
I can hear the good earth groaning
crushed beneath a billion souls
just seeking their century
salvation in wealth.

And so the modern world goes
as Gaia sighs and turns to stone
to wait upon a wiser age
when sages and keepers
will come once again.

Beyond Mere Support –

In Service of Dreams

Colleagues
called to be keepers