Selection and Use of Reference Materials for Establishing Traceability

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Selection and Use of Reference Materials for Establishing *Quality*

I'll be discussing issues surrounding this… which is in fact different!

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Traceability isn't Quality

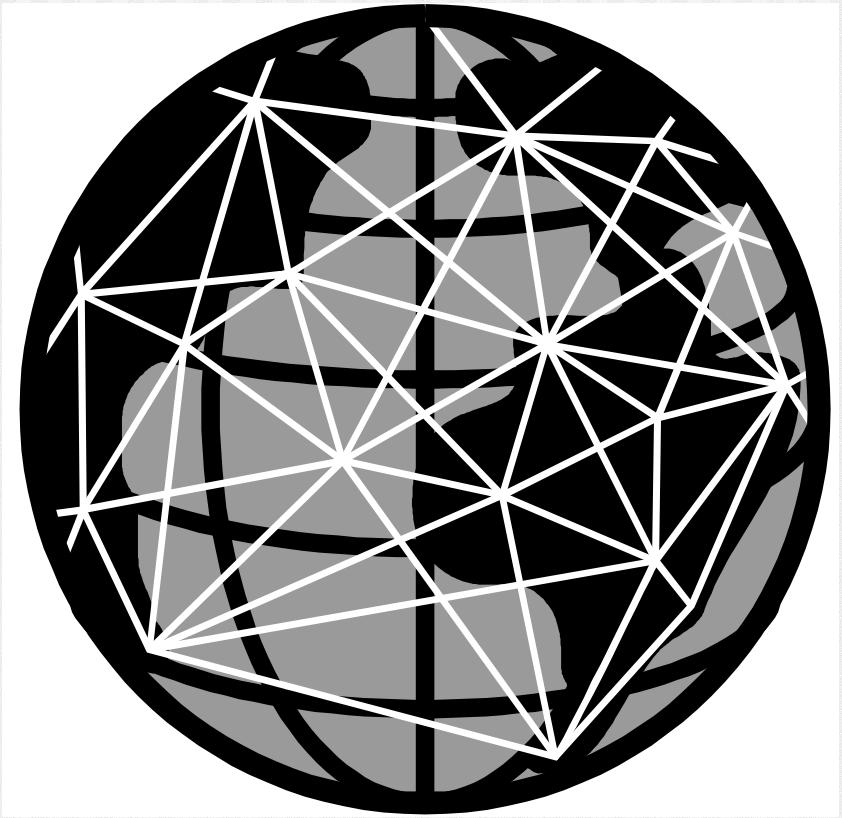
- traceability isn't an umbrella under which we can hide
  - it's *part* of quality
- being traceable, even to a good reference, doesn't mean you're right!
- *all it does is let us compare results*

Comparing results

- results are only useful when compared
  - to other results
    - e.g., to observe a trend
  - to limits
    - e.g., a threshold for action
  - different results in different places or measured at different times…
    - *"comparability over space-and-time"*

Comparability of results

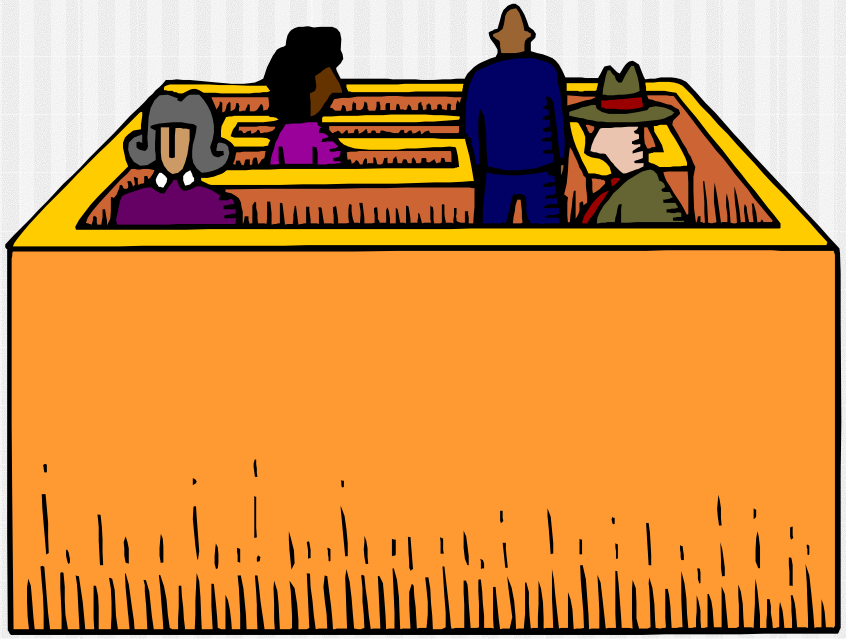
- Whole and sole goal of traceability.
  - *raison d'être!*
- results linked to a common reference can be compared
- scope of reference defines scope of comparability
  - global network
    - SI



“But traceability in chemistry is different!”

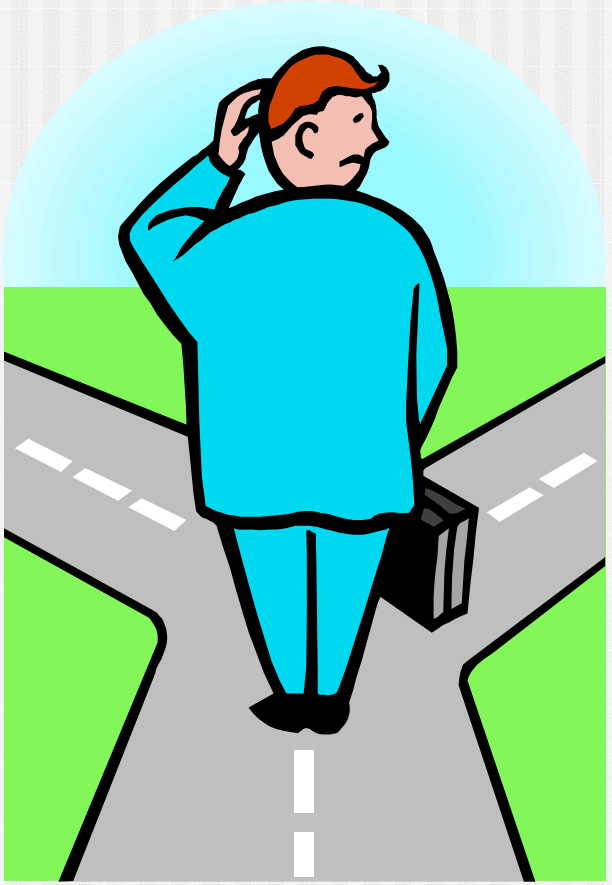
- “…formidable difficulties exist in establishing international traceability for measurements in chemistry.”

  20th Conférence Générale des Poids et Mesures, 1995



Traceability in chemistry…

- is different.
  - identity
    - what am I measuring, anyway?
  - interference
    - do I get the same response for analyte in my calibration material and in it's matrix?
  - morphology
    - is the analysis the same everywhere in my sample?



Traceability in chemistry…

- is different.
  - the fallacy is that valid methods have…
    - defined scope
    - clear measurement model
      - assure that the analyte is what's being measured
      - robustness w.r.t. interference

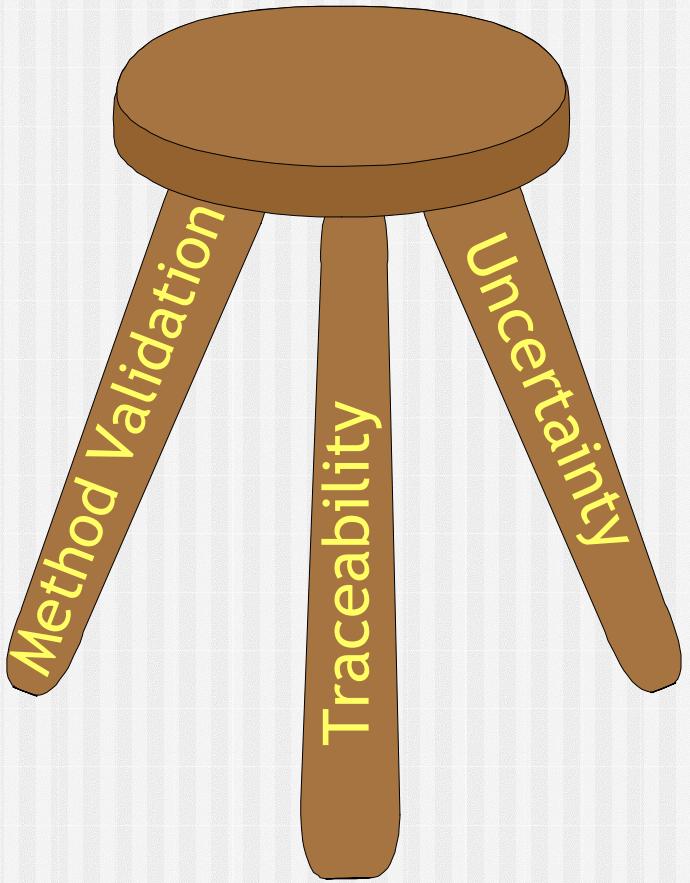
Measurement model

$$C_{Unknown} = \frac{C_{Standard}}{S_{Standard}} S_{Unknown}$$

- if you get this part right…
  - you've demonstrated that…
    - you know what you're measuring
    - it's not affected by other stuff
  - you know how to keep your method in control

“Quality” in Chemical Measurements

- method validation
  - am I measuring what I set out to measure?
- uncertainty
  - how well do I know the result of what I’ve measured?
- traceability of result
  - can I compare this result with other results?

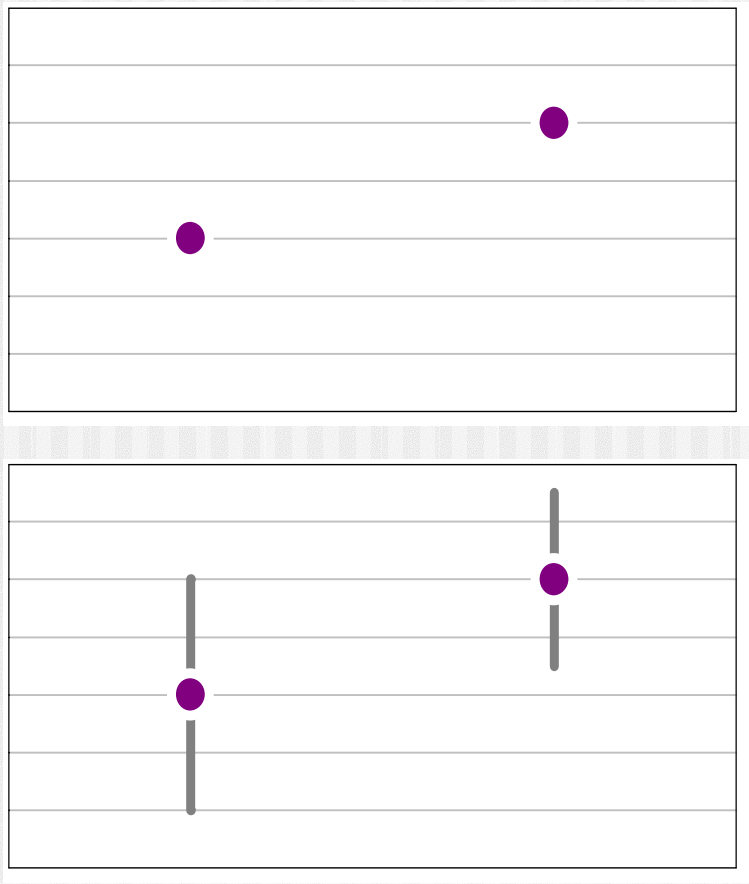


Method validation

- checks the model
  - tests completeness
  - tests assumptions
  - helps establish an uncertainty budget
- identifies relevant parameters to keep under control
- tests scope

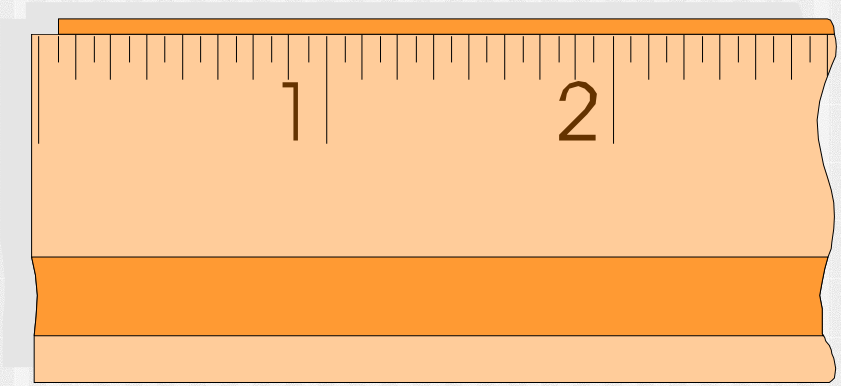
Uncertainty budget

- how well do you know the result?
  - essential part of being able to compare!
    - are these two results the same???
- are these results good enough?
  - fit-for-purpose



Traceability

- *Traceability* is how you get units on your result
  - in our simple model, convert from units of your measurement tool to units of the 'standard'
- *'standards' may appear in several places in model!*
  - where 'correction' is required
    - *'recovery'*

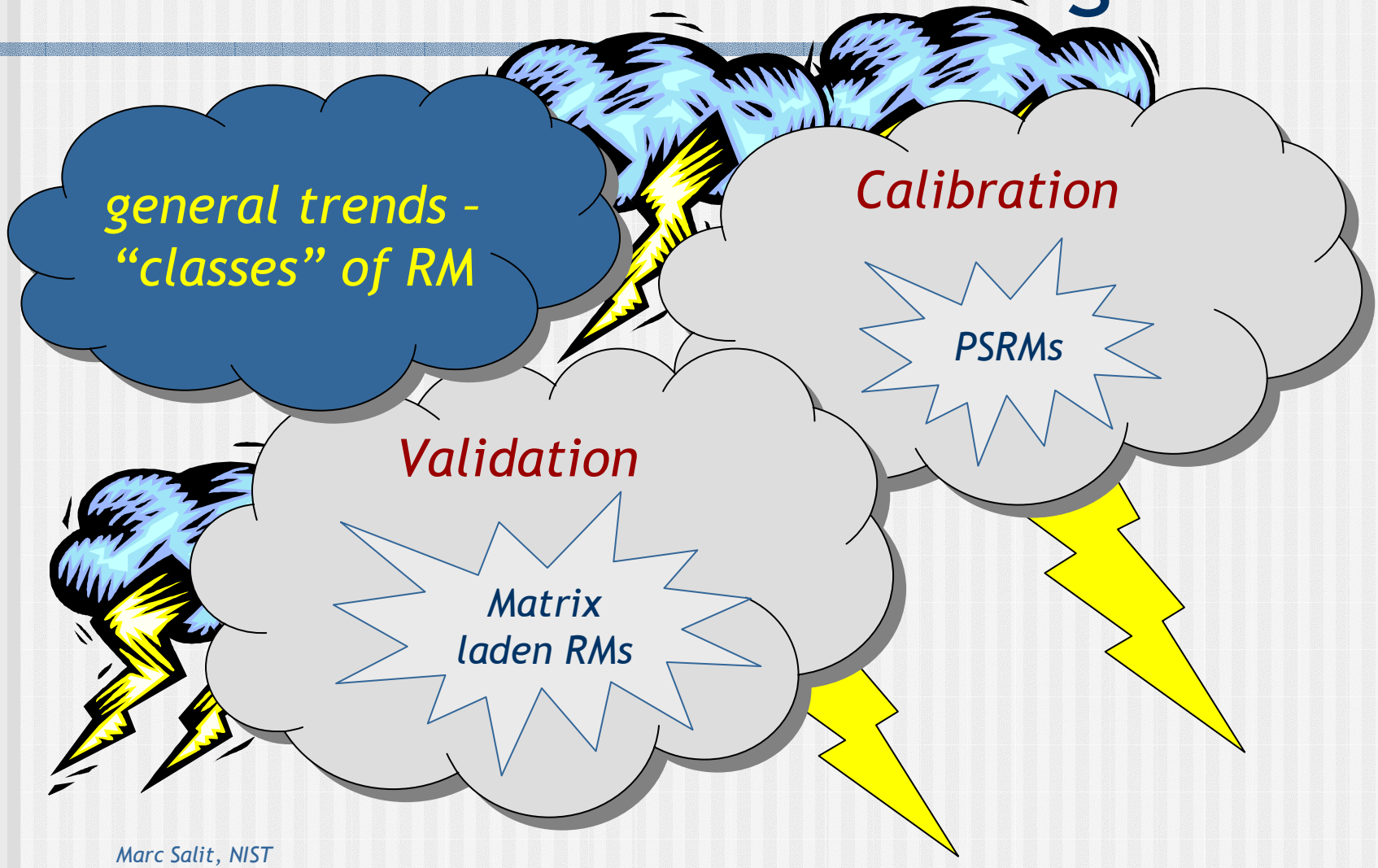


$$C_{Unknown} = \frac{C_{Standard}}{S_{Standard}} S_{Unknown} \cdot \left(\frac{Added}{Found} \right)$$

Roles of reference materials

- method validation
  - test the model
- uncertainty
  - evaluate bias
  - control charting
    - *need stability, not certified value!*
- traceability
  - common references

Reference material usage…



CRMs for method validation

- "I ran a CRM, and…
  - I got the right answer."
    - useful i… there…
  - I got the answer."
    - also useful information here!

remember what method validation is doing…

Method validation

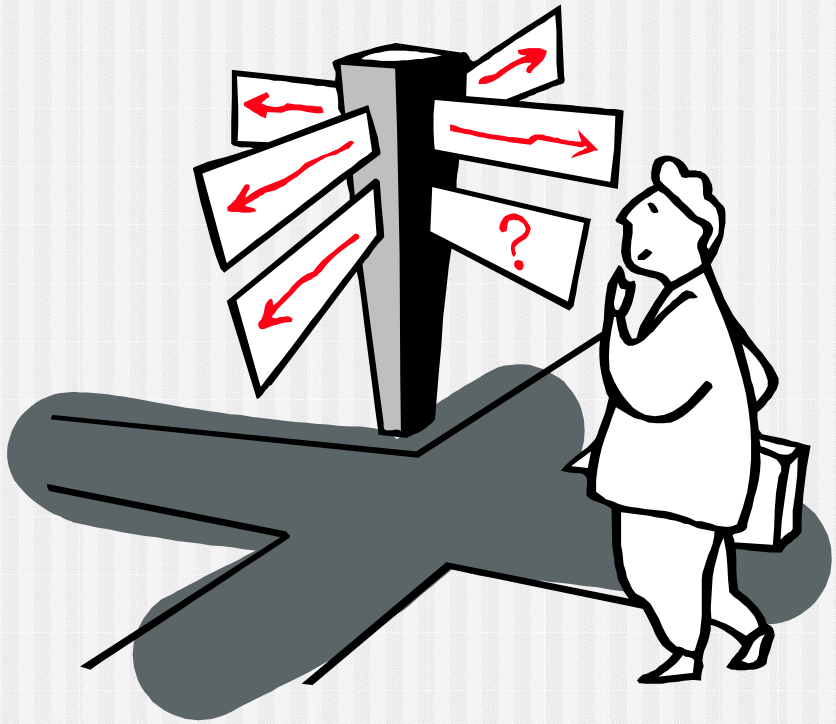
- checks the model
  - tests completeness
  - tests assumptions
  - helps establish an uncertainty budget
- identifies relevant parameters to keep under control
- tests scope

CRMs for method validation

- establish ‘quality’ of measurement
  - deploy method with known performance
  - use series/”suite” of CRMs to establish scope
    - *‘How far does the light shine?’*
- *CRMs play vital role in chemistry*

RMs for validation

- good selection requires understanding of…
  - chemistry of the sample
  - chemistry of the validation material
  - physics of the measurement

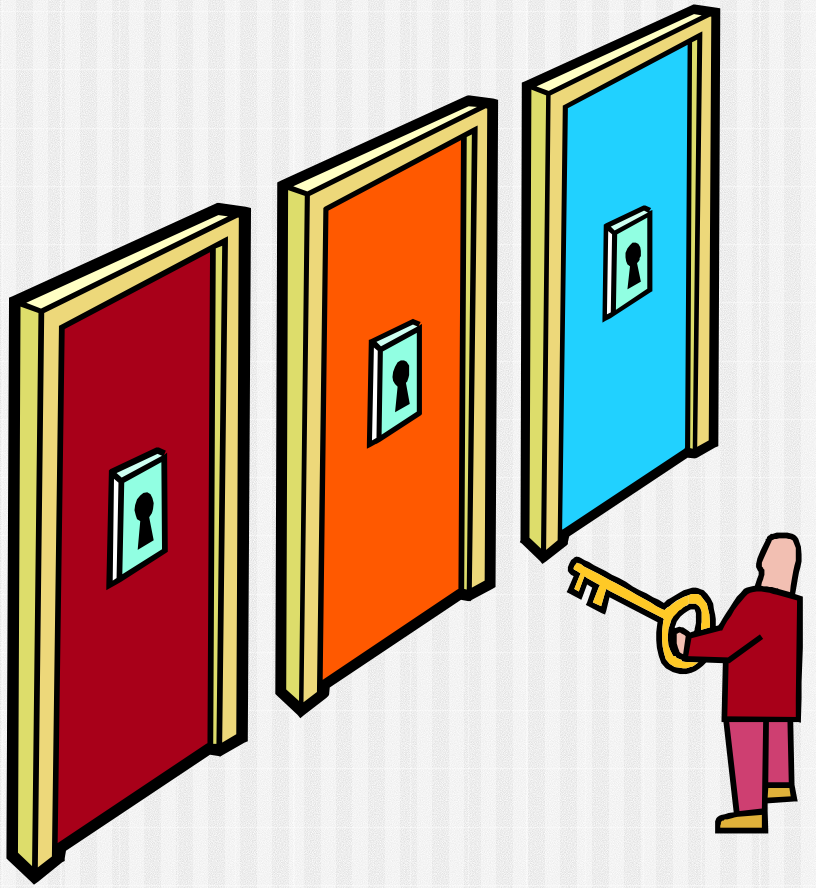


Calibration materials

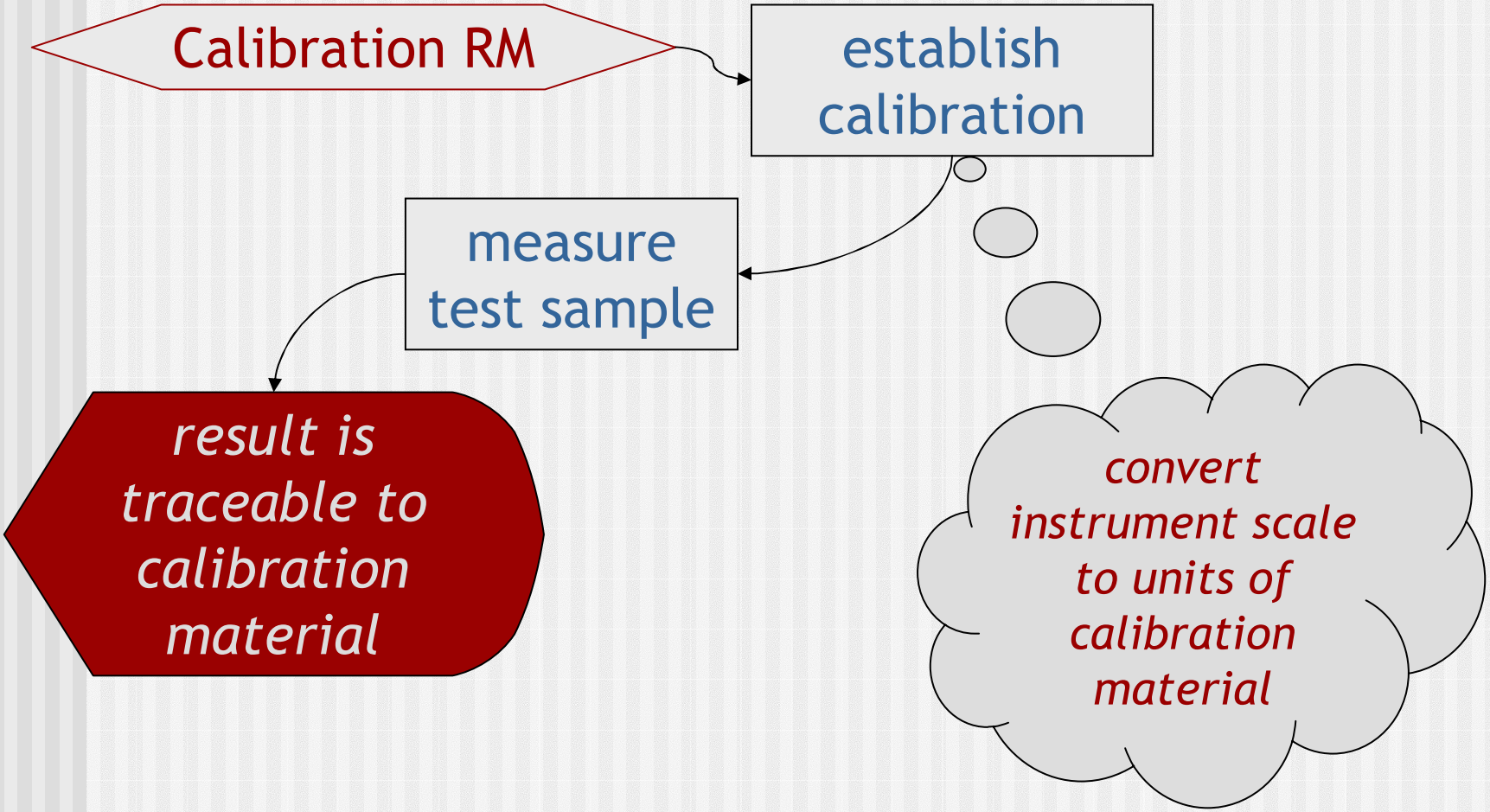
- *traceability of reference determines scope of traceability of results!*
  - local traceability gives local comparability
  - global traceability gives global comparability
- PSRMs traceable to SI
  - *global scope!*
  - purity determination
    - source of value
    - source of uncert.

Calibration materials

- PSRMs
  - no matrix
    - applicable to many…
  - reagent grade materials often suitable
    - fit-for-purpose
- require knowledge…
  - physics
  - chemistry of PSRM
  - chemistry of sample
- regulatory compliance
  - may require **CRM**
  - may require scope



Establishing Traceability…



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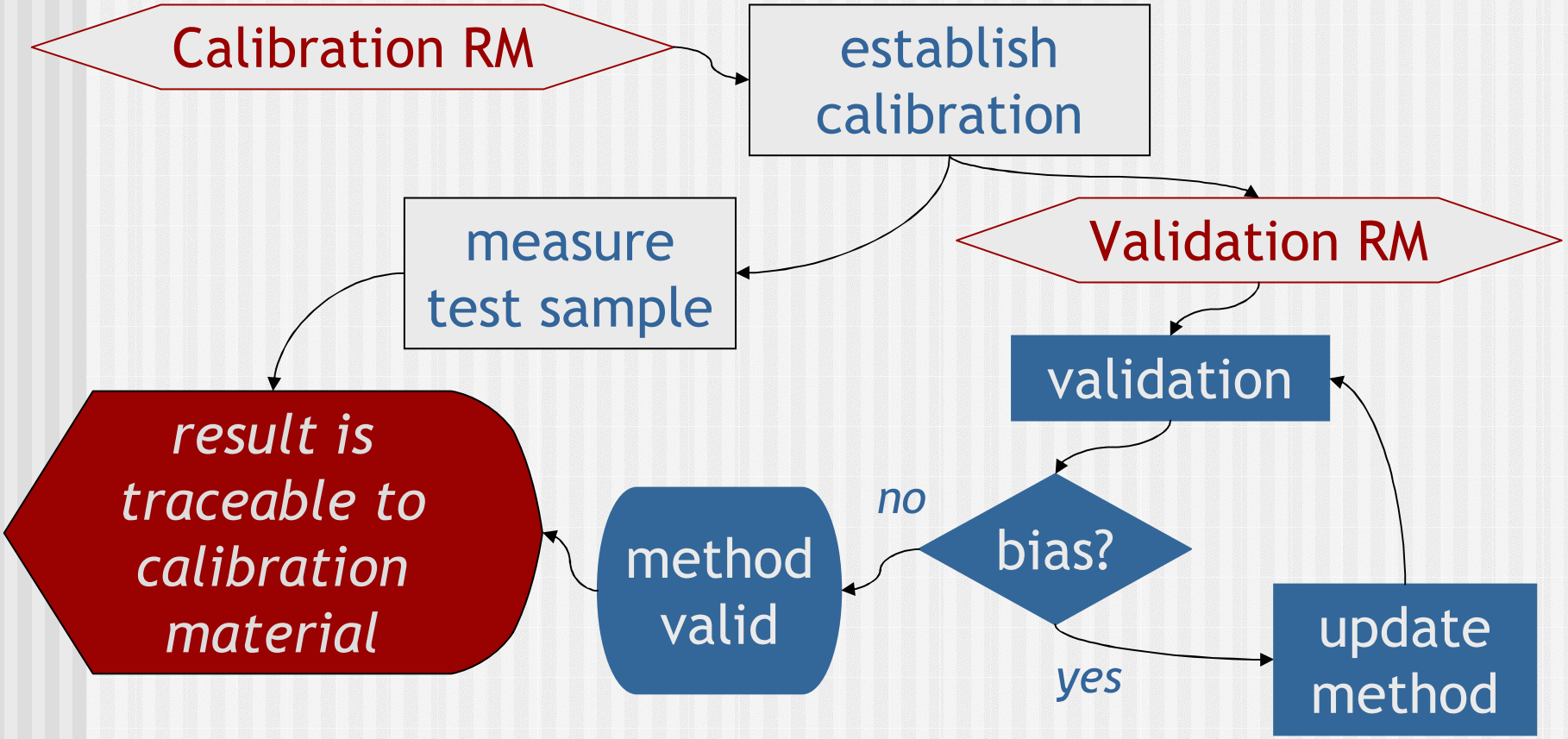

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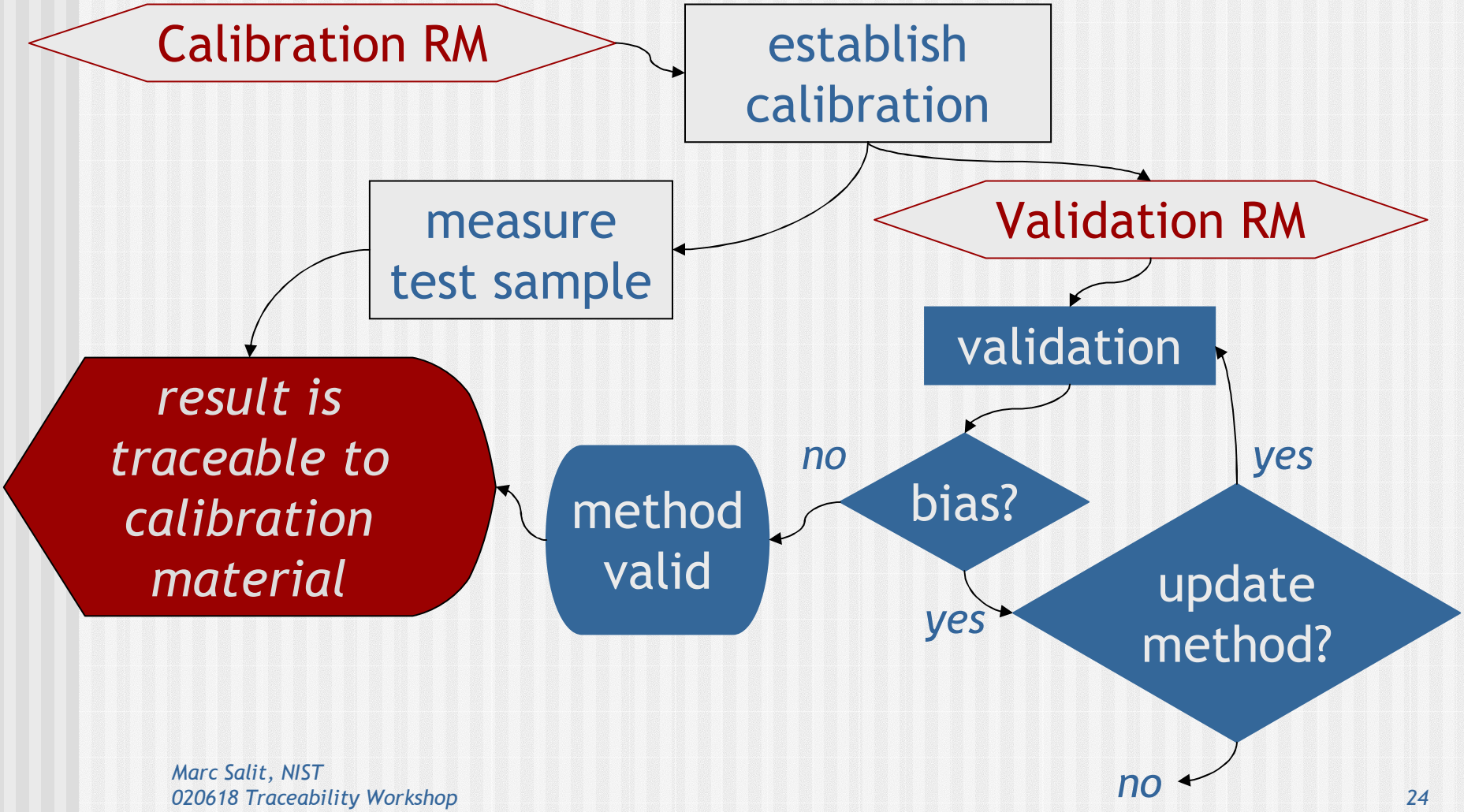

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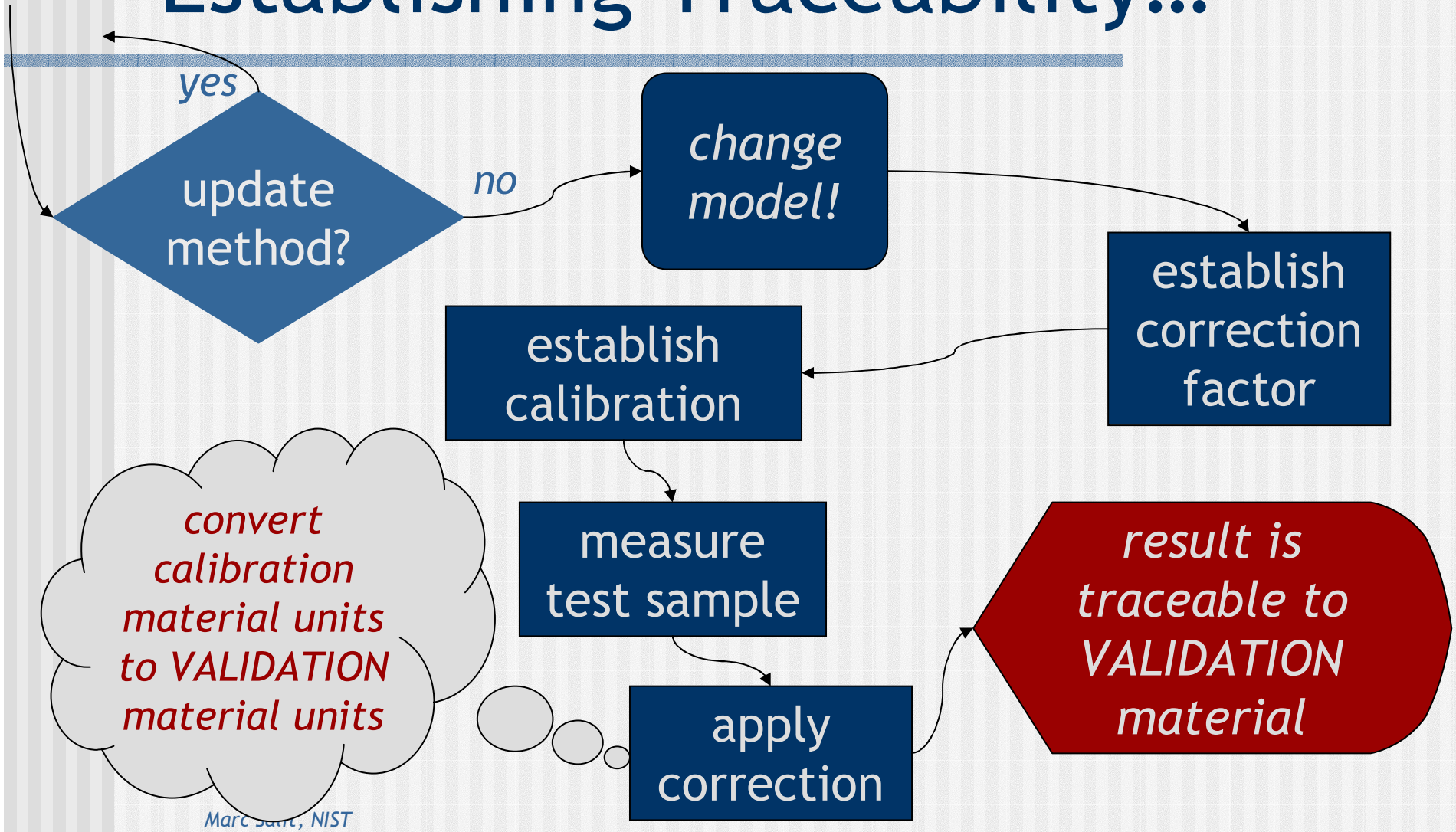

Matrix CRMs *v.* PSRMs

- Matrix CRMs
  - leverage the best measurements!
    - expensive, high-effort techniques to certify
    - information xfer to less expensive tools
  - matrix-match?
  - uncertainty
    - fit-for-purpose?
    - homogeneity?
  - *is traceability to these good enough?*
- PSRMs
  - small uncertainty
    - often stable
    - homogeneous
    - no morphology
  - realization of the kilogram or the mole
    - traceability to SI
  - purity determination often very certain
  - more easily reproduced
  - more easily deployed
  - *needs valid method!*

As analytical science progresses…

- matrix-indifferent methods
  - less need for CRMs
- intrinsic standards
  - use data for calibration
    - spectroscopy
      - *quantum stds?*
- self-validating methods
  - *PSRM calibration procedure validates and gives traceability*