Lecture 3
Nuclear Data

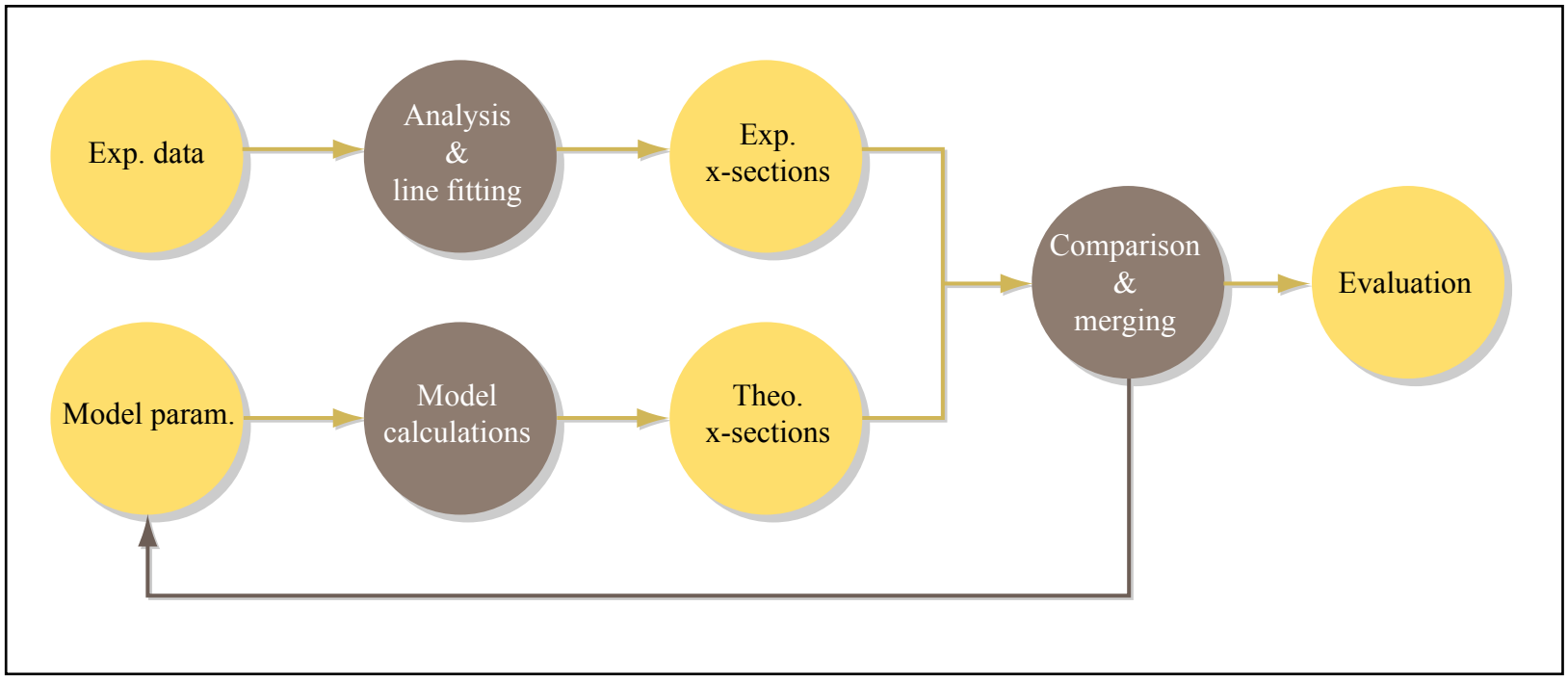
22.106 Neutron Interactions and Applications

Spring 2010

Common Misconceptions

- It’s just a “bunch” of numbers
- Just give me the right value and stop changing it.

Traditional evaluation method



Theoretical model

- Computer code SAMMY
  - Used for analysis of neutron and charged particle cross-section data
  - Uses Bayes method to find parameter values
    - Generalized least squares
  - Uses R-matrix theory to tie experimental data to theoretical models
    - Reich-Moore approximation
    - Breit-Wigner theory
  - Treats most types of energy-differential cross sections
    - Treats energy and angle differential distributions of scattering
  - Fits integral data
  - Generates covariance and sensitivity parameters for resolved and unresolved resonance region

Three energy regions

- Resolved resonance range
  - Experimental resolution is smaller than the width of the resonances; resonances can be distinguished. Cross-section representation can be made by resonance parameters
  - R-matrix theory provides for the general formalism that are used

- Unresolved energy range
  - Cross-section fluctuations still exist but experimental resolution is not enough to distinguish multiplets. Cross-section representation is made by average resonance parameters
  - Formalism
    - Statistical models e.g. Hauser-Feshbach model combined with optical model
    - level density models, ….
    - Probability tables

The Unresolved Resonance Range (URR)

- Energy range over which resonances are so narrow and close together that they cannot be experimentally resolved.
- A combination of experimental measurements of the average cross section and theoretical models yields distribution functions for the spacings and widths.
- The distributions may be used to compute the 'dilute-average' cross sections:

$$\left\langle \sigma_s(E) \right\rangle = \sum_l \left[\frac{4\pi}{k^2}(2l+1)\sin^2\varphi_l + \frac{2\pi^2}{k^2}\sum_J \left(\frac{g_J}{\left\langle D_{l,J} \right\rangle} \left\langle \frac{\Gamma_{n,l,J}^2}{\Gamma_{l,J}} \right\rangle - 2\left\langle \Gamma_{n,l,J} \right\rangle \sin^2\varphi_l \right) \right]$$

$$\left\langle \sigma_c(E) \right\rangle = \sum_l \frac{2\pi^2}{k^2}\sum_J \frac{g_J}{\left\langle D_{l,J} \right\rangle} \left\langle \frac{\Gamma_{n,l,J}\Gamma_{\gamma,l,J}}{\Gamma_{l,J}} \right\rangle$$

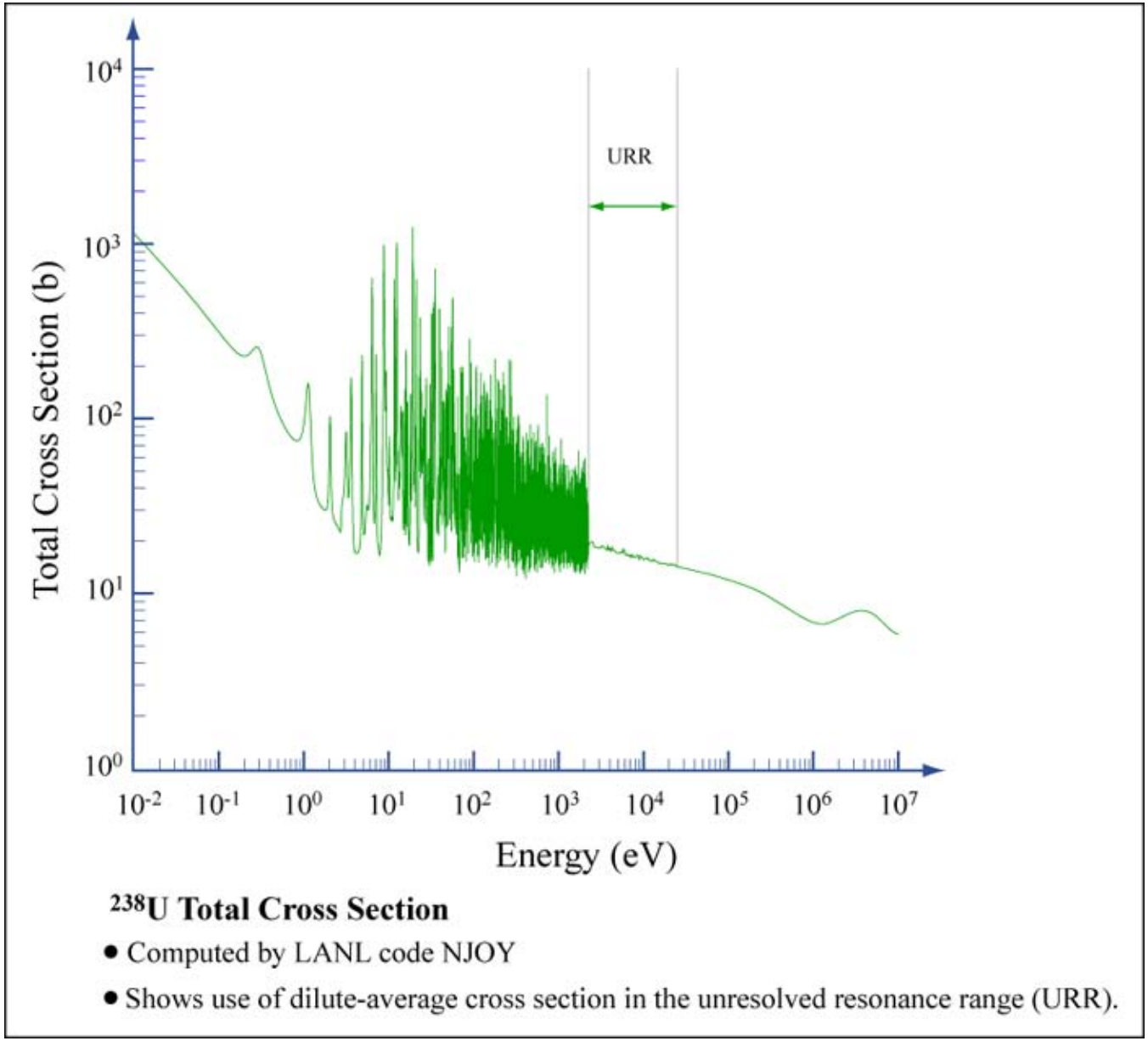
$$\left\langle \sigma_f(E) \right\rangle = \sum_l \frac{2\pi^2}{k^2}\sum_J \frac{g_J}{\left\langle D_{l,J} \right\rangle} \left\langle \frac{\Gamma_{n,l,J}\Gamma_{f,l,J}}{\Gamma_{l,J}} \right\rangle$$

l = orbital angular momentum quantum no., J = spin of the compound nucleus

k = wave number, g_J = spin statistical factor, φ_l = phase shift

$\Gamma_{n,l,J}$, $\Gamma_{\gamma,l,J}$, $\Gamma_{f,l,J}$, $\Gamma_{l,J}$ = neutron, capture, fission, and total widths

$D_{l,J}$ = resonance spacing, $\langle \cdots \rangle$ denotes averaging over the distribution(s)



^{238}U Total Cross Section

- Computed by LANL code NJOY
- Shows use of dilute-average cross section in the unresolved resonance range (URR).

The Probability Table Method

- Concept developed in the early 1970s by Levitt (USA) and Nikolaev, *et al*. (USSR).
- Uses the distributions of resonance widths and spacings to infer distributions of cross section values.
- Basic idea:
  - Compute the probability p_n that a cross section in the URR lies in band n defined as $\hat{\sigma}_{n-1} < \sigma \leq \hat{\sigma}_n$.
  - Compute the average value of the cross sections (σ_n) for each band n.
  - Following every collision (or source event) in a Monte Carlo calculation for which the final energy of the neutron is in the URR, sample a band-averaged cross section with the computed probabilities and use that value for that neutron until its next collision.

Mathematical Theory of the Probability Table Method

- $p_t(\sigma, E)d\sigma \equiv$ probability that the total cross section lies in $d\sigma$ about σ at energy E
- Average total cross section: $\langle \sigma_t(E) \rangle = \int d\sigma \, \sigma \, p_t(\sigma, E)$
- Band probability: $p_n(E) = \int_{\hat{\sigma}_{n-1}}^{\hat{\sigma}_n} d\sigma \, p_t(\sigma, E)$
- Band-average total cross section: $\sigma_{t,n}(E) = \dfrac{1}{p_n(E)} \int_{\hat{\sigma}_{n-1}}^{\hat{\sigma}_n} d\sigma \, \sigma \, p_t(\sigma, E)$
- $q_\alpha(\sigma', E|\sigma)d\sigma' \equiv$ conditional probability that the partial cross section of type α lies in $d\sigma'$ about σ' given that the total cross section has the value σ
- Band-average partial cross section: $\sigma_{\alpha,n}(E) = \dfrac{1}{p_n(E)} \int_{\hat{\sigma}_{n-1}}^{\hat{\sigma}_n} d\sigma \, p_t(\sigma, E) \int_0^{\sigma} d\sigma' \, q_\alpha(\sigma', E|\sigma)$

Unfortunately, computing $p_t(\sigma, E)$ *and* $q_\alpha(\sigma', E|\sigma)$ *directly is an intractable problem.*

Monte Carlo Algorithm for Generating the Tables

- Use ENDF/B parameters to create probability distribution functions (PDFs) for resonance widths (Wigner distribution) and spacings (chi-squared distributions).
- Randomly sample widths and spacings from PDFs to generate 'fictitious' sequences (realizations) of resonances about the energy *E* for which the table is being created.
- Use single-level Breit-Wigner formulae to compute sampled cross section values at E:

$$\sigma_s(E) = \sigma_{s,\,\text{smooth}}(E) + \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\varphi_l + \frac{4\pi}{k^2}\sum_l\sum_J g_J \sum_{r\in R_{lJ}} \frac{\Gamma_{nr}}{\Gamma_r}\left\{\left[\cos(2\varphi_l) - \left(1 - \frac{\Gamma_{nr}}{\Gamma_r}\right)\right]\psi(\theta_r, X_r) - \sin(2\varphi_l)\chi(\theta_r, X_r)\right\}$$

$$\sigma_\alpha(E) = \sigma_{\alpha,\,\text{smooth}}(E) + \frac{4\pi}{k^2}\sum_l\sum_J g_J \sum_{r\in R_{lJ}} \frac{\Gamma_{nr}\Gamma_{\alpha r}}{\Gamma_r^2}\psi(\theta_r, X_r),\ \alpha = \text{c, f}$$

$\sigma_{\alpha,\text{smooth}}$ = tabulated background cross section, α = s, c, f

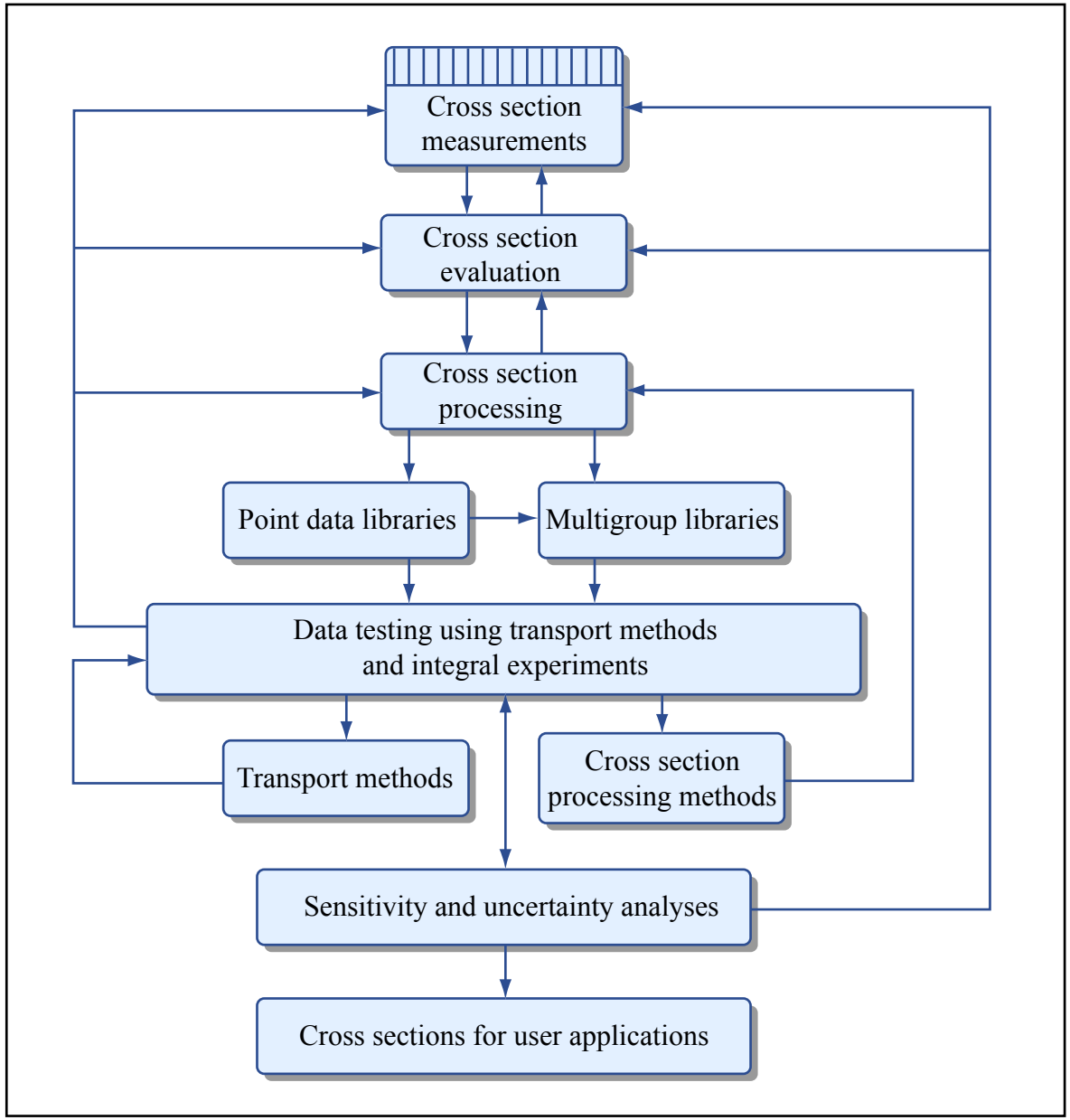
$\Gamma_{n,r}, \Gamma_{\gamma,r}, \Gamma_{f,r}, \Gamma_r$ = neutron, capture, fission and total widths for resonance *r*

R_{lJ} = set of sampled resonances for quantum number pair (*l*,*J*)

ψ, χ = Doppler functions, $\theta_r \equiv \Gamma_r / \sqrt{4k_B TE/A}$, $X_r \equiv 2(E - E_r)/\Gamma_r$, A = atomic mass

- Use the sampled cross sections to compute band averages and probabilities.

- High energy region
  - No cross-section fluctuations exist. Cross-sections are represented by smooth curves.
  - Formalism
    - Statistical models e.g. Hauser-Feshbach
    - Intra-nuclear cascade model
    - Pre-equilibirum model
    - Evaporation model



ORELA

- High flux (10^{14} n/s)
- Excellent Resolution (Δt = 2-30 ns)
  - faciliates better evaluations
- “White” neutron spectrum from 0.01eV to 80 MeV
  - Reduces systematic uncertainties
- Measurement systems and background well understood
  - Very accurate data
- Simultaneous measurements in different beams lines
- Measurements performed on over 180 isotopes

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ORELA Target

- High energy electrons hitting a tantalum target produce bremsstrahlung (photon) spectrum. Neutrons are generated by photonuclear reactions, Ta(gamma, n), Ta(gamma, 2n), …

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Bayesian Inference

- Bayesian inference is statistical inference in which evidence or observations are used to update or to newly infer what is known about underlying parameters or hypotheses.

Cost of evaluations

Single iteration (min):	Assumptions (for single 3GHz PC):
Model calculations: 400 X 50 X 2 X 20 = 800 000	400 nuclides
Benchmark parameter-sensitivity: 400 X 50 X 2 X 500 = 20 000 000	50 parameters/nuclide
Library Benchmarking: 400 000	Single model calculation (1 nuclide up to 20 MeV - 20 min)
Total: ~ 21 000 000 min = 40 years	Benchmark sensitivity to a single parameter 500 min
	Full library benchmark 400 000 min
1 iteration per week - 2100 CPU's	

Covariance Matrix

- The covariance matrix or dispersion matrix is a matrix of covariances between elements of a random vector. It is the natural generalization to higher dimensions of the concept of the variance of a scalar-valued random variable.

$$\Sigma = \begin{bmatrix} \mathrm{E}[(X_1 - \mu_1)(X_1 - \mu_1)] & \mathrm{E}[(X_1 - \mu_1)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_1 - \mu_1)(X_n - \mu_n)] \\ \mathrm{E}[(X_2 - \mu_2)(X_1 - \mu_1)] & \mathrm{E}[(X_2 - \mu_2)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_2 - \mu_2)(X_n - \mu_n)] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{E}[(X_n - \mu_n)(X_1 - \mu_1)] & \mathrm{E}[(X_n - \mu_n)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_n - \mu_n)(X_n - \mu_n)] \end{bmatrix}$$

- Each type of data comes from a separate measurement
  - Cross-sections are measured independently
  - However, the various types are highly interrelated
- Data include measurement-related effects
  - Finite temperature
  - Finite size of samples
  - Finite resolution
  - …
- Measured data may look very different from the underlying true cross-section
  - Think Doppler broadening

Advantages of evaluated data

- Incorporate theoretical understanding
  - Cross-section shapes
  - Relationships between cross-sections for different reactions
- Incorporate all available experimental data and all available uncertainty
- Allow extrapolation
  - Different temperatures
  - Different energies
  - Different reactions

- Generate artificial “experimental” points from ENDF resonance parameters
  - Include Doppler and resolution broadening
- Make reasonable assumptions regarding experimental uncertainties
  - Statistical (diagonal terms)
  - Systematic (off-diagonal terms)
    - Normalization, background, broadening, …

- Run models with varying resonance parameters with an assumed distribution
- Include systematic uncertainties for measurement-related quantities
- Perform simultaneous fit to all data
  - All experimental uncertainty is thus propagated

Computational cost

- Large cases require special care
  - U-235 has ~3000 resonances
    - 5 parameters for each resonance need to be varied
    - Very time consuming

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