MICHIGAN STATE UNIVERSITY

ABACUS: A Bayesian-Delphi Framework for Plasma Transport Coefficients

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Transport Coefficients are Increasingly Important

- At high temperatures, transport is more important: the plasma is more kinetic.
- How do we assign confidence in our knowledge in the values of the transport coefficients?

Black is Euler hydrodynamics; color extends to generalized Navier-Stokes.

$$\frac{\partial n_\alpha}{\partial t} + \nabla \cdot (n_\alpha \mathbf{v}) = \nabla \cdot (D_\alpha \nabla n_\alpha)$$

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho(\mathbf{v} \cdot \nabla)\mathbf{v} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g}$$

$$\rho_e \frac{\partial e_e}{\partial t} + \rho_e(\mathbf{v} \cdot \nabla)e_e = -p_e(\nabla \cdot \mathbf{v}) + \nabla \cdot (k_e \nabla T_e) + Q_{ei}$$

$$\rho_i \frac{\partial e_i}{\partial t} + \rho_i(\mathbf{v} \cdot \nabla)e_i = -p_i(\nabla \cdot \mathbf{v}) + \nabla \cdot (k_i \nabla T_i) + \boldsymbol{\tau} : \nabla \mathbf{v} - Q_{ei}$$

We wish to know the uncertainty in transport coefficient (TC) X at state $\mathbf{x}$:

$$X(\mathbf{x}) = \bar{X}(\mathbf{x}) + \Delta X(\mathbf{x})$$

$$\mathbf{x} = (T, \rho, Y_1, ..., Y_k)^\top$$

1. Choose the best model
2. Do sensitivity analysis on that model

$$\boldsymbol{\tau} = \eta \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T - \frac{2}{3}(\nabla \cdot \mathbf{v})\mathbf{I} \right) + \zeta (\nabla \cdot \mathbf{v})\mathbf{I}$$

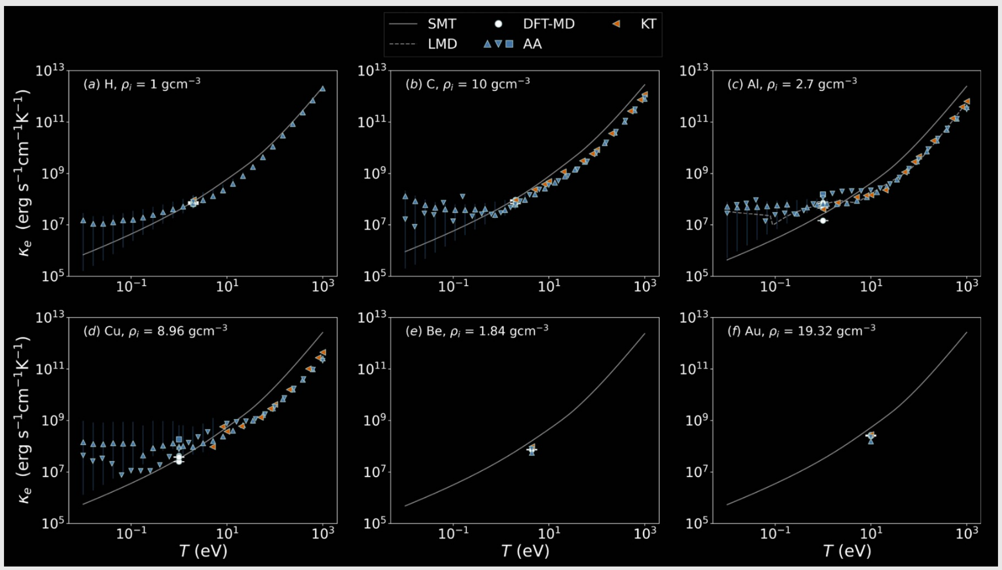
The viscous stress tensor depends on the shear and bulk viscosities.

$$\frac{dE_\alpha}{dx} = -\frac{4\pi Z_\alpha^2 e^4 n_e \ln \Lambda}{m_e v_\alpha^2}$$

Alpha particles are completely kinetic and are handled differently.

Transport Model Comparisons

Workshops in 2020 and 2024 explored a wide range of models across wide ranges of materials, temperatures, densities and processes/coefficients.



ELSEVIER
High Energy Density Physics
Volume 37, November 2020, 100905

Review of the first charged-particle transport coefficient comparison workshop

P.E. Grabowski [a], S.B. Hansen [b], M.S. Murillo [c], L.G. Stanton [d], F.R. Graziani [a], A.B. Zylstra [a], S.D. Baalrud [f], P. Arnault [g], A.D. Baczewski [b], L.X. Benedict [a], C. Blancard [h], O. Čertík [e], J. Clérouin [g], L.A. Collins [e], S. Copeland [a], A.A. Correa [a], J. Dai [i], J. Daligault [e], M.P. Desjarlais [b], M.W.C. Dharma-wardana [j]...A. White [e]

RESEARCH ARTICLE | MAY 02 2024

Review of the second charged-particle transport coefficient code comparison workshop

Special Collection: Charged-Particle Transport in High Energy Density Plasmas

Lucas J. Stanek; Alina Kononov; Stephanie B. Hansen; Brian M. Haines; S. X. Hu; Patrick F. Knapp; Michael S. Murillo; Liam G. Stanton; Heather D. Whitley; Scott D. Baalrud; Lucas J. Babati; Andrew D. Baczewski; Mandy Bethkenhagen; Augustin Blanchet; Raymond C. Clay, III; Kyle R. Cochrane; Lee A. Collins; Amanda Dumi; Gerald Faussurier; Martin French; Zachary A. Johnson; Valentin V. Karasiev; Shashikant Kumar; Meghan K. Lentz; Cody A. Melton; Katarina A. Nichols; George M. Petrov; Vanina Recoules; Ronald Redmer; Gerd Röpke; Maximilian Schörner; Nathaniel R. Shaffer; Vidushi Sharma; Luciano G. Silvestri; François Soubiran; Phanish Suryanarayana; Mikael Tacu; Joshua P. Townsend; Alexander J. White

$$\mathcal{M} = \{m_1, m_2, \ldots, m_K\}$$

Models were diverse: kinetic theory, average atom, MD, density functional theory, etc.

Standard Model Selection (Data Science)

Model selection is a formal process for considering a set of candidate models $\mathcal{M}$ and choosing the best one using data.

But what does "best" mean?

A model that fits the data well but has many parameters may be overfitting; a parsimonious model may underfit. The best model balances goodness-of-fit against complexity.

Criteria such as the AIC (Akaike Information Criterion) and BIC (Bayesian Information Criterion) quantify this tradeoff.

$$\text{AIC} = 2k - 2\ln(\hat{L})$$

$$\text{BIC} = k\ln(n) - 2\ln(\hat{L})$$

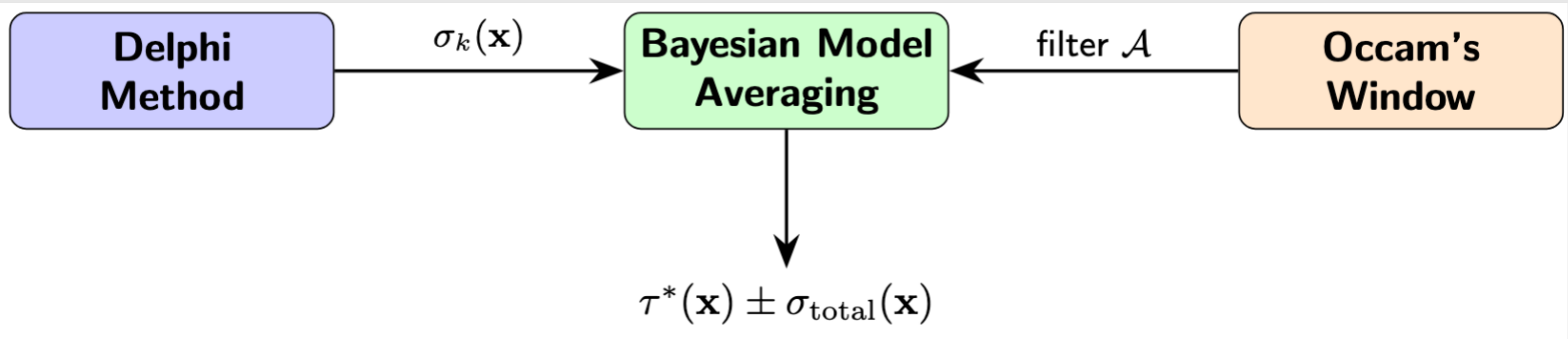
- **AIC** applies a fixed penalty of 2 per parameter. It is grounded in information theory—specifically, it approximates the Kullback-Leibler divergence between the fitted model and the unknown true distribution. AIC tends to favor more complex models and is aimed at finding the best predictive model.

- **BIC** penalizes by *ln(n)* per parameter, so the penalty grows with sample size. It derives from a Bayesian perspective as an approximation to the log marginal likelihood (model evidence). BIC is more conservative and tends to select simpler models, especially for large *n*.

ABACUS Roadmap

ABACUS = Averaged Bayesian Approach Combining Uncertainty and Subjectivity

The Problem:
- There is no best model to select.
- We have sparse experimental data in extreme regimes.
- Human insight can carry more weight than equations.



Component	Purpose	Provides
Bayesian Model Averaging	Principled model combination	Weighted estimates + total variance
Delphi Method	Elicit expert knowledge	Prior probabilities + uncertainties
Occam's Window	Manage model complexity	Focused model subset

Bayesian Model Averaging (BMA): The Mathematical Framework

Consider the set M of K models: $\mathcal{M} = \{m_1, m_2, \ldots, m_K\}$ with data D

The probability the transport coefficient has value τ is given by an average over all models.

$$p(\tau|\mathcal{D}, \mathbf{x}) = \sum_{k=1}^{K} p(\tau|\mathcal{D}, m_k, \mathbf{x}) \cdot p(m_k|\mathcal{D}, \mathbf{x})$$

The expected value τ^* of the transport coefficient is obtained from:

$$\mathbb{E}[\tau|\mathbf{x}] = \int \tau \cdot p(\tau|\mathcal{D}, \mathbf{x})\, d\tau$$

$$\begin{aligned} \tau^* &= E[\tau|\mathbf{x}] \\ &= \sum_{k=1}^{K} E[\tau|m_k, \mathbf{x}] \cdot p(m_k|\mathcal{D}, \mathbf{x}) \end{aligned}$$

Variances in BMA

$$\mathrm{Var}(\tau|\mathbf{x}) = \underbrace{E[\mathrm{Var}(\tau|m_k)]}_{\text{within-model}} + \underbrace{\mathrm{Var}(E[\tau|m_k])}_{\text{between-model}}$$

$$E[\mathrm{Var}(\tau|m_k)] = \sum_{k=1}^{K} \sigma_k^2(\mathbf{x}) \cdot p(m_k|\mathbf{x})$$

$$\mathrm{Var}(E[\tau|m_k]) = \sum_{k=1}^{K} (E[\tau|m_k] - E[\tau])^2 \cdot p(m_k|\mathbf{x})$$

$$E[\tau] = \sum_{k=1}^{K} E[\tau|m_k] \cdot p(m_k|\mathbf{x})$$

We have a Major Problem!

HEDP transport coefficient data is extremely sparse in temperature-density-species space.

Mathematically, the

$$p(\mathcal{D}|m_k, \mathbf{x})$$

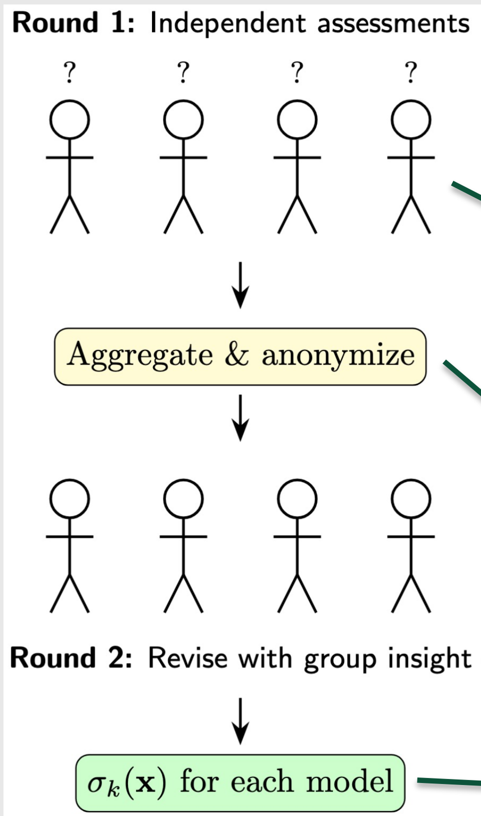
are very poorly known.

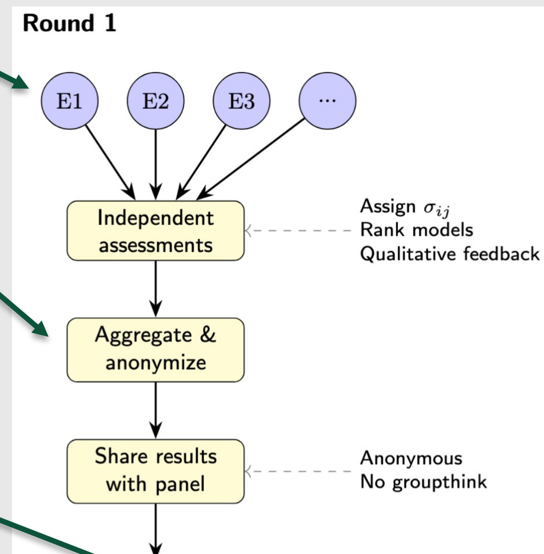
This is particularly acute for HEDP applications that span variations in $\boldsymbol{x}$ beyond known datasets.

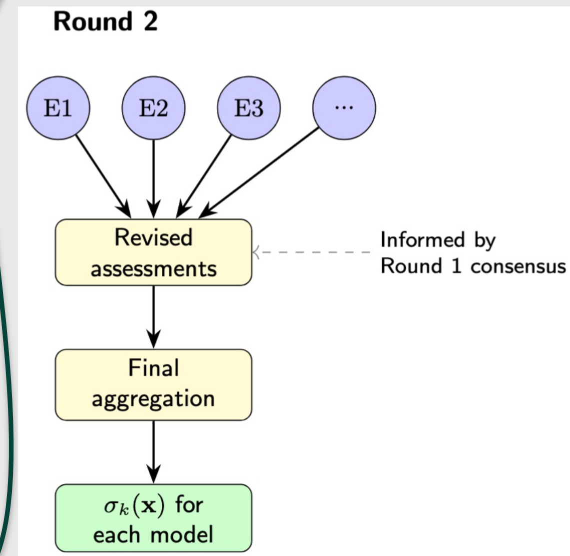
How do we assign uncertainty to a model in the complete absence of data?

The Delphi Method: Structured Expert Consensus

RAND Corporation, 1950s: How do you forecast when data doesn't exist? Ask experts — but avoid groupthink.





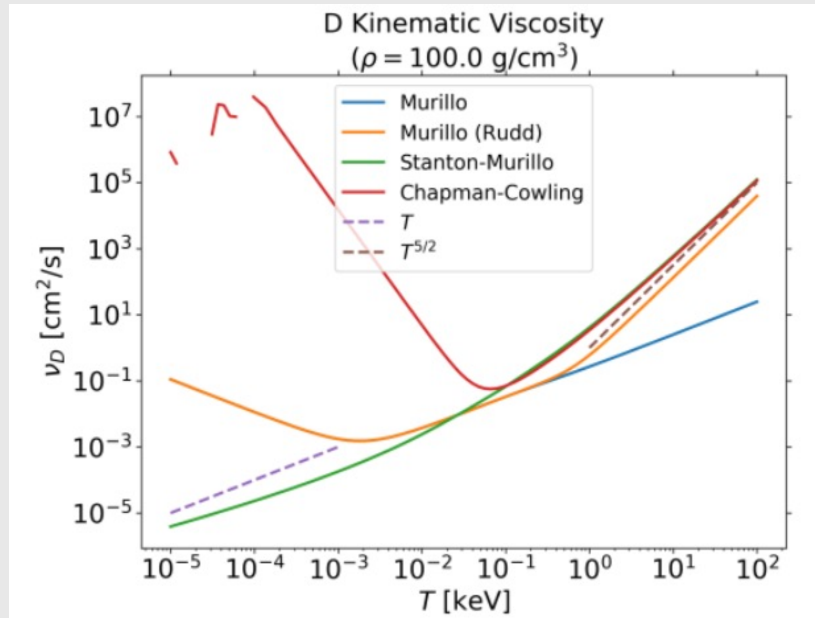


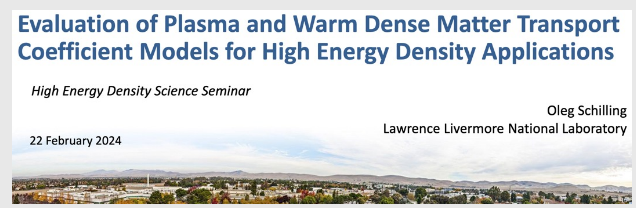
Occam's Window

Some models should not be included.

In fact, certain *classes* of models might be ruled out:

- use incorrect interparticle potentials
- Neglect quantum mechanics
    - atomic physics (e.g., MIS)
    - diffractive scattering
    - Pauli exclusion





Delphi Prompts

For these $\mathcal{S}$ plasma states,

(1) rank and window the models,

$$\mathcal{S} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_L\} \quad \mathcal{M}' = \left\{m_k : \frac{p(m_k|\mathcal{D},\mathbf{x})}{\max_j p(m_j|\mathcal{D},\mathbf{x})} > c\right\}$$

(2) assign an uncertainty to the models,

$$\Sigma^2 = \{\sigma_1^2, \sigma_2^2, \ldots, \sigma_L^2\}$$

(3) discuss your logic

ABACUS: Integrating BMA with Expert Knowledge

$$p(m_k|\mathbf{x}) = \frac{\exp(-\lambda \cdot \text{rank}_k(\mathbf{x}))}{\sum_{j=1}^{K} \exp(-\lambda \cdot \text{rank}_j(\mathbf{x}))}$$

Method 1

$$p(m_k|\mathbf{x}) = \frac{1/\sigma_k(\mathbf{x})}{\sum_{\ell=1}^{K} 1/\sigma_\ell(\mathbf{x})}$$

Method 2

ABACUS Prediction(s)

Rankings: $$p(m_k|\mathbf{x}) = \frac{e^{-\lambda\,\mathrm{rank}_k}}{\sum_\ell e^{-\lambda\,\mathrm{rank}_\ell}}$$

Uncertainties: $$p(m_k|\mathbf{x}) = \frac{1/\sigma_k}{\sum_\ell 1/\sigma_\ell}$$

Combined: $$p(m_k|\mathbf{x}) = \frac{e^{-\lambda\,\mathrm{rank}_k}/\sigma_k^2}{\sum_\ell e^{-\lambda\,\mathrm{rank}_\ell}/\sigma_\ell^2}$$

$$\tau^*(\mathbf{x}) = \sum_{k\in\mathcal{A}} p(m_k|\mathbf{x}) \cdot \mathbb{E}[\tau|m_k, \mathbf{x}]$$

Summary and Discussion

The Problem:

- ~18 TCCW models, order-of-magnitude disagreements
- Sparse experimental data in extreme regimes
- How to choose? How to quantify uncertainty?

Component	Role
BMA	Principled weighted averaging
Delphi	Expert-derived $\sigma_k(x) \rightarrow p(m_k \mid x)$
Occam's Window	Exclude inapplicable models

Contact me!
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Back-up Slides

BMA: Three Intuitive Approximations

Prior Dominates (weak data): $p(m_k|\mathcal{D}, \mathbf{x}) \approx p(m_k|\mathbf{x})$

$$\tau^* \approx \sum_{k=1}^{K} \mathbb{E}[\tau|m_k, \mathbf{x}] \cdot p(m_k|\mathbf{x})$$

Type II MAP: $\tau^* \approx \mathbb{E}[\tau|m_{\mathrm{MAP}}, \mathbf{x}]$

$$m_{\mathrm{MAP}} = \arg\max_{m_k} p(m_k|\mathcal{D}, \mathbf{x})$$

$$p(m_k|\mathcal{D}, \mathbf{x}) = \frac{p(\mathcal{D}|m_k, \mathbf{x}) \cdot p(m_k|\mathbf{x})}{\sum_{j=1}^{K} p(\mathcal{D}|m_j, \mathbf{x}) \cdot p(m_j|\mathbf{x})}$$

Type II MLE: $\tau^* \approx \mathbb{E}[\tau|m_{\mathrm{MLE}}, \mathbf{x}]$

$$m_{\mathrm{MLE}} = \arg\max_{m_k} p(\mathcal{D}|m_k, \mathbf{x})$$

Special Case: K=2

$$p(m_1|\mathcal{D},\mathbf{x}) = \frac{p(\mathcal{D}|m_1,\mathbf{x})}{p(\mathcal{D}|m_1,\mathbf{x}) + p(\mathcal{D}|m_2,\mathbf{x})}$$

$$p(m_1|\mathcal{D},\mathbf{x}) = \frac{\mathrm{BF}_{12}}{\mathrm{BF}_{12}+1} \equiv \mathcal{B}$$

$$\mathrm{BF}_{12}(\mathbf{x}) = \frac{p(\mathcal{D}|m_1,\mathbf{x})}{p(\mathcal{D}|m_2,\mathbf{x})}$$

Special Case: K=2

$$\tau^*(\mathbf{x}) = \mathcal{B} \cdot \mathbb{E}[\tau|m_1] + (1-\mathcal{B}) \cdot \mathbb{E}[\tau|m_2]$$

$$\mathrm{Var}(\tau|\mathcal{D},\mathbf{x}) = \underbrace{\mathcal{B}\,\sigma_1^2 + (1-\mathcal{B})\,\sigma_2^2}_{\text{within-model}} + \underbrace{\mathcal{B}(1-\mathcal{B})(\mu_1-\mu_2)^2}_{\text{between-model}}$$

Table 1: Limiting behavior of the two-model BMA estimate.

BF_{12}	$\mathcal{B}$	Result
$\to \infty$	$\to 1$	$\tau^* \to \mathbb{E}[\tau|m_1]$ (model 1 dominates)
$= 1$	$= \frac{1}{2}$	$\tau^* = \frac{1}{2}\big(\mathbb{E}[\tau|m_1] + \mathbb{E}[\tau|m_2]\big)$ (equal weight)
$\to 0$	$\to 0$	$\tau^* \to \mathbb{E}[\tau|m_2]$ (model 2 dominates)

Table 2: Physical interpretation of between-model variance in the two-mo case.

Scenario	Between-model variance
$\mathcal{B} = \frac{1}{2}$ (models equally supported)	Maximum
$\mathcal{B} \to 0$ or $\mathcal{B} \to 1$ (one model dominates)	Zero
$\mu_1 \approx \mu_2$ (models agree)	Small
$\mu_1 \neq \mu_2$ (models disagree)	Large

Limiting Cases

No data, equal priors:

$$\tau^* = \frac{1}{K}\sum_{k=1}^{K} \tau_k, \quad \sigma^2 = \frac{1}{K}\sum_{k=1}^{K}(\tau_k - \tau^*)^2$$

With expert weights only:

$$\tau^* = \sum_{k=1}^{K} w_k \tau_k, \quad \text{where} \quad w_k = \frac{1/\sigma_k^2}{\sum_j 1/\sigma_j^2}$$

BIC: Bayesian Information Criteria

$$p(\mathcal{D}|m_k) = \int p(\mathcal{D}|\theta_k, m_k) \cdot p(\theta_k|m_k)\, d\theta_k$$

$$\ln p(\mathcal{D}|m_k) \approx \ln p(\mathcal{D}|\hat{\theta}_k, m_k) - \frac{d_k}{2} \ln n$$

$$\mathrm{BIC} = -2 \ln p(\mathcal{D}|\hat{\theta}_k, m_k) + d_k \ln n$$

Agreement Metric

Kendall's W measures agreement:

$$W = \frac{12\sum_{k=1}^{K}\left(R_k - \bar{R}\right)^2}{N^2(K^3 - K)}$$

W	Interpretation
0	No agreement (random)
0.1–0.3	Weak agreement
0.3–0.5	Moderate agreement
0.5–0.7	Good agreement
0.7–0.9	Strong agreement
1	Perfect agreement

Symbol	Definition
R_k	Sum of ranks for model k across all experts
$\bar{R}$	Expected mean rank sum $= \frac{N(K+1)}{2}$
N	Number of experts
K	Number of models

Example:

Model	Expert 1	Expert 2	Expert 3	Row Sum R_k
m_1	1	2	1	4
m_2	3	3	4	10
m_3	2	1	2	5
m_4	4	4	3	11