

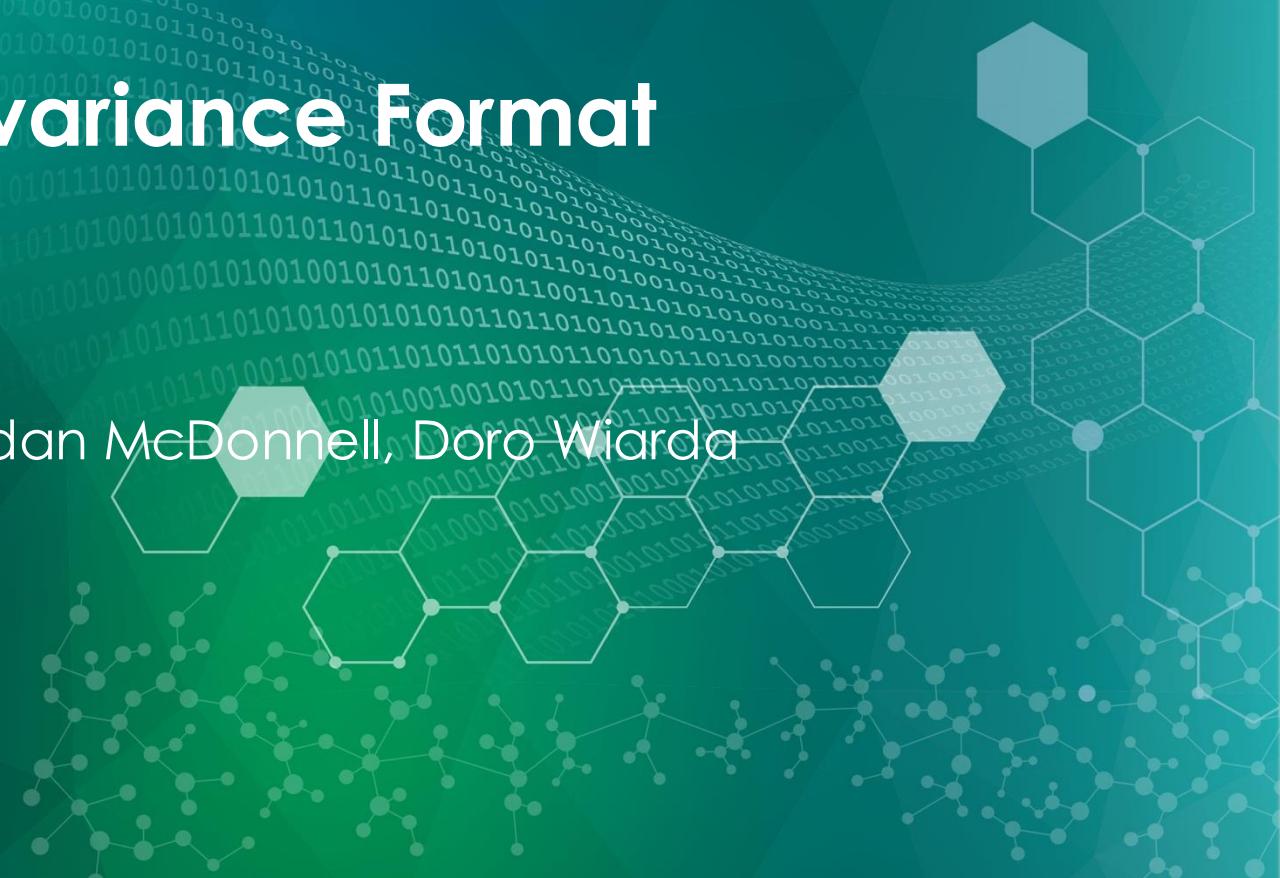
Progress on MF37: TSL Covariance Format

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Current Progress

- MF37/MT4 Incoherent Inelastic Covariance $S(\alpha, \beta)$
 - Option for storing 2 different quantities:
 - Covariance of phonon density of states (PDOS), bound scattering cross section
 - Covariance of $S(\alpha, \beta)$, bound scattering cross section, effective temperature
 - Each option has pros and cons, can leave up to evaluator to determine best implementation for material
 - PDOS more compact, but potential loss of physical features
 - $S(\alpha, \beta)$ more exact, but needs reduction to be usable
 - Efforts underway to determine best practices for evaluators

Next Steps

- Currently: 1 temperature for MF37/MT4
- Goal: arbitrary temperatures for MF37/MT2 & MF37/MT4
 - Ambitious, but doable
- MF37/MT2 (incoherent & coherent elastic)
 - Incoherent:
 - Scalar quantity (Debye-Waller) as a function of temperature; mathematically straightforward
 - Coherent:
 - Energy-dependent quantity as a function of temperature; computationally straightforward

Open Questions

- Temperature Effects
 - Incoherent Elastic: straightforward
 - Coherent Elastic: possible, see below
 - Incoherent Inelastic: difficult, might rely on effective temperature
- MF37/MT2 (coherent elastic)
 - Can be described entirely using the Debye-Waller factor (W) if no desire for temperature-dependent Bragg scattering
 - Current CE implementation involves sampling scattering energy/angle; less intuitive on how covariance would be implemented

To Do

- MF37/MT4:
 - 1 temperature light water covariance work nearing completion (see talk tomorrow)
 - Multiple temperature implementation ongoing
- MF37/MT2:
 - Need to identify potential candidate materials (contingent on MF37/MT4 above)
 - Covariance generation would be similar to light water MF37/MT4
- Everything:
 - Next CSEWG?!?

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