COUPLING THERMODYNAMIC COMPUTATIONS WITH MULTI-PHYSICS NUCLEAR FUEL CODES

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A new equilibrium thermodynamic solver called Thermochimica has been developed with the primary purpose of direct integration into multi-physics codes. In particular, the software is intended to provide various material properties and boundary conditions to the Advanced Multi-Physics (AMP) nuclear fuel performance code. The development of Thermochimica in this research is aimed at addressing several concerns with using commercially available software, including: licensing entanglements associated with code distribution, access to the source code, convenient incorporation into other codes with quality assurance considerations, and computational performance. In particular, significant research efforts have been dedicated to enhance computational performance through advanced algorithm development, such as improved estimation techniques and non-linear solvers. The overall goal of this undertaking is to provide a computational tool to enhance the predictive capability of multi-physics codes without significantly impeding computational performance.

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