High temperature causes several adverse effects in modern-day chips, adversely affecting the chip's performance and reliability. It also increases the leakage power, which further increases the on-chip temperature, resulting in a feedback effect. State-of-the-art works in thermal estimation have serious limitations in modeling some important effects contributing to temperature. Additionally, these methods are slow. We overcome the limitations of these works by developing fast Green's function-based analytical methods. Such methods have been shown to be faster than the traditional finite difference and finite element methods, but their use has been limited to simple problems in the past. In this thesis, we develop Green's function-based methods for a wide range of complex thermal problems and demonstrate their superior efficiency compared to existing works. In the first work, we developed a fast and analytical leakage-aware thermal simulator for 3D chips using Green's functions. Next, we extend this work to compute the thermal profile for 3D chips with microchannels by taking care of the anisotropicity in the thermal profile of such chips. In the next work, we propose an analytical thermal simulator that considers the effects of process variation, temperature-dependent conductivity, and temperature-dependent leakage power altogether. However, an analytical process variation-aware method cannot be extended to complex geometries. So, in our final work, we propose a convolutional neural network architecture for thermal estimation in the presence of variability that leverages the physics of heat transfer. In summary, by using a combination of rare mathematical transforms, algebraic manipulations, and numerical and machine learning-based methods, we not only solve these complex problems but also achieve greater than 100X speedup over the state-of-the-art simulators with comparable accuracy in all of our works. Thus, the work presented in this thesis significantly advances the state-of-the-art in ultra-fast thermal estimation.