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Eleven carefully selected, peer-reviewed contributions from the Virtual Conference on Computational Science (VCCS-2016) are featured in this edited book of proceedings. VCCS-2016, an annual meeting, was held online from 1st to 31st August 2016. The theme of the conference was "Computational Thinking for the Advancement of Society" and it matched the paradigm shift in the way we think. VCCS-2016 was attended by 100 participants from 20 countries. The chapters reflect a wide range of fundamental and applied research applying computational methods.
