Extreme Scale Computing, Big Data Science and Web-of-Life Network Science

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ABSTRACT

I will motivate the presentation on extreme scaling as a unifying theme in extreme scale computing, big data science and the web-of-life.

In the first part of the presentation I will explore two leading formal models of concurrency in computer science, the polyhedral and CSP, as a distinct approach to extreme scale computing.

In the second part I will present three grand challenge areas as exemplars of extreme scale big data science: environmental science (climate modelling), genomics life science (tree of life) and computational neuroscience (deep learning). Here the underlying scaling characteristics are energy-efficiency, resilience and predictive capability. I will highlight some current research which explores distance minimisation, self-organising and asynchronous data flow computational principle for extreme scale data science.

The final part is a curiosity driven exploratory research under the "theoretical computer science meets biological phenomena" premise that radical advancements in deep measurements of all life on this planet is bringing two grand biological phenomena into the realms of computer science and with deep computations at the extreme scales offers new avenues for a big data science from productive cross-collaboration between the sciences. I will highlight some computational principles to investigate this grand goal of modelling the eco-system continuous dynamics of "web of life" to account for "information domain" (network dynamics) of biological phenomena along with matter and energy. Networks permeate all scales of life — from genes to the web of life.

I will conclude with some pointers on the multi-disciplinary partnerships necessary to systematically map the scientific challenges at the interface of Computer Science and Big Data Sciences to establish general principles for data driven scientific advancements.

Bio

Dr. Manjunathaiah has a long standing track record in computer science, computational science, data science research and education from positions held at: Harvard University USA (visiting Assistant Professor of Computational Science at IACS, in the Harvard John A. Paulson School of Engineering and Applied Sciences in September 2017) and in the U.K. at University of Oxford (Research fellowship), University of Manchester (Research fellowship), University of Southampton (Commonwealth Scholar), School of Mathematical, Physical and Computational Sciences at the University of Reading in the U.K. (Lecturer in Computational Science), School of Engineering and Computer Science, University of Hertfordshire (Senior Lecturer) and from collaborating with leading international research groups (INRIA, IRISA, Colorado) in parallel and concurrent computation and exascale computing (ANL, NERSC).

Dr. Manjunathaiah's research interests span theoretical and practical computer science in parallel and concurrent computing, as well as interdisciplinary areas in computational and data science to advance solutions to grand challenge problems: Climate Science (Exascale Climate models) and Computational Biology (Big data Phylogeny). His research experience is in two prominent formalisms in parallelism and concurrency in Computer Science: Polyhedral Model and CSP, parallel architectures, parallelising compilers, parallel program verification, hardware-software co-design, performance modelling on Petascale systems, and domain specific programming languages to explore parallel and concurrent computations in various domains.

Dr. Manjunathaiah's interests are driven by a 'curiosity' of what is computable and the phenomena of computation itself. In particular he is interested in computation as a modelling means to answer the fundamental question: 'does nature behave in this way' ? He has taught extensively covering foundations of Computer Science (Discrete Maths), core areas (Algorithms, OS, Compilers) and advanced topics (Concurrent Systems) and he received the faculty of science award for 'outstanding contribution to teaching and learning' at the University of Reading in 2007.