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Here and now: the intersection of computational science and computer science

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Quantum-mechanical simulations have become dominant and widely used tools for scientific discovery and technological advancement; since they are performed without any experimental input or parameter they can streamline, accelerate, or replace actual physical experiments. This is a far-reaching paradigm shift, substituting the cost- and time-scaling of brick-and-mortar facilities, equipment, and personnel with those, very different, of computing engines.

Nevertheless, computational science remains anchored to a renaissance model of individual artisans gathered in a workshop, under the guidance of an established practitioner. Great benefits could follow from rethinking such model, while adopting concepts and tools from computer science for the automation, management, preservation, analytics, and dissemination of these computational efforts.

I will offer my perspective on the current state-of-the-art in the field, its power and limitations, and the role and opportunities of high-throughput computing (HTC, rather than HPC), of open source codes and workflows, and of big data available on demand.

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