



The relentless march of Moore's law



This special edition of the *Journal* showcases recent work in metallurgical applications of computational modelling. But what exactly is computational modelling? Historically this would have included any science or engineering problem that required a computer to solve numerical approximations of the governing equations. Computers were typically large, expensive pieces of equipment, and the problems solved were limited by the available power of the machine – early applications included chemical thermodynamics, numerical heat and mass transfer, and simple problems in fluid flow.

However, in modern times we have computing pervading our lives to an ever-increasing degree, and we are starting to catch more unusual fish in our computational modelling nets. Driven by sustained exponential growth in computer power over more than six decades (your wristwatch today has more capability than was available to the entire Apollo space programme), methods such as computational fluid dynamics have been enhanced beyond all recognition and are now capable of modelling realistic engineering problems with multiphase flow and free surface interfaces, coupled heat transfer, electromagnetic fields, and others. Tools like massively-parallel GPU accelerators are also breathing new life into old methods like discrete element modelling, giving us unprecedented insight into particulate flow problems.

Alongside the rapid growth in capability and performance of traditional computational modelling tools, the role of such models in the knowledge industry has also evolved. From being able to give an isolated (and usually not very accurate) result, they are now routinely used to study the general behaviour of systems across wide ranges of their parameter spaces. Such models are also increasingly viewed as intermediate analysis and interpretation tools for building intuition rather than producing the 'final answer', and they generate one thing that is in short supply in metallurgical processes – data. And since data feeds the physics-informed or data-driven reduced order models which power the ongoing revolution in artificial intelligence, computational modelling will remain a useful piece of the puzzle for a long time to come.

Q.G. Reynolds

*Pyrometallurgy Division, Mintek
Chemical Engineering Department, Stellenbosch University*