Vectorised non-spherical particle models for discrete element computations

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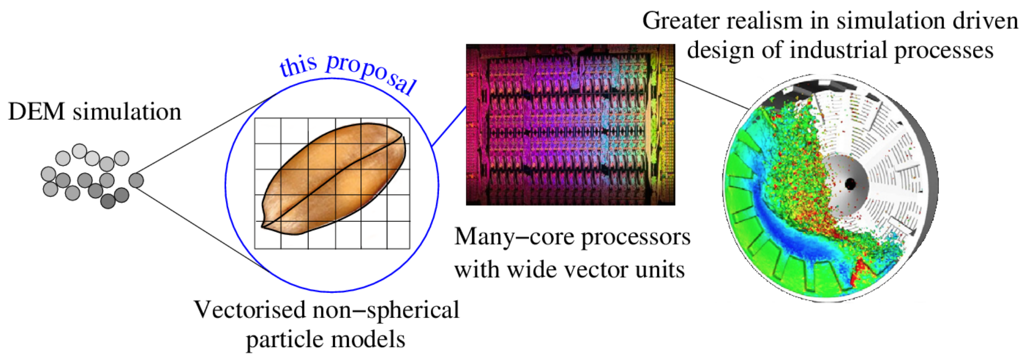

Figure 1. Discrete Element Method (DEM) [1] equipped with efficient non-spherical particle models optimised for modern compute cores (e.g. Xeon Phi) will offer a greater realism in simulation driven design of industrial processes (e.g. comminution [8]).

Background

Computers these days become faster via becoming multi-core (several compute cores per processor) or many-core (tens or hundreds of compute cores per processor/accelerator). Individual compute cores do not become faster, rather the opposite. Nonetheless, individual cores are accompanied by increasingly more powerful *vector units*. Vector units allow to evaluate certain algebraic and analytical operations all at once for a batch of input variables that are suitably aligned in computer memory. As a result, the compute power of current computers can be summarised as follows:

compute power = many cores + vector operations on each core.

Contact detection in DEM algorithms takes advantage of parallel processing by executing multiple particle to particle contact detection (P2PCD) tests concurrently. Nonetheless, individual P2PCD tests do not scale any further. Although several non-spherical particle models have been proposed in the DEM literature, e.g. [2-7], none of them have been designed with an explicit understanding of how efficiency is achieved on contemporary computer architectures. Consequently, these models do not immediately lend themselves to an efficient implementation on cores equipped with vector units, or briefly, to *vectorisation*. Given the existing trend in the evolution of the computational hardware, this represents a significant gap in the current DEM research, ignorance of which may lead to a significant loss of opportunity in the future.

This proposal

This proposal seeks to bridge the *vectorisation gap* in the research on non-spherical DEM particle models. This is not only important for the present industrial applications, but is also a precondition for DEM being able to enter the era of exascale computing with an offering going beyond computing on spheres. Consequently, our aims in this proposal are threefold:

- Review of existing non-spherical particle models from the point of view of suitability for vectorisation (a top down approach),
- Development of new particle models strictly aligned to the emerging many-core hardware architectures (a bottom up approach),
- Donation into the public domain of a minimalist software library of highly optimised P2PCD tests between a variety of non-spherical particle models (dissemination).

The results of our work, in the form of the P2PCD software library, will be available without any restrictions to academic and industrial users (MIT license). In its spirit, it will aim to replicate in the field of DEM computing, what libraries such as BLAS or LAPACK did in the field of dense linear algebra (becoming de facto standards).

References

[1] P.A. Cundall, O.D.L. Strack, Geotechnique, 29 (1979) 47-45.
[2] J.F. Ferellec, G.R. McDowell, Granular Matter, 12 (2010) 459-467.
[3] E.G. Nezami, Y.M.A. Hashash, D. Zhao, J. Ghaboussi, Computers and Geotechnics, 31 (2004) 575-587.
[4] C.W. Boon, G.T. Houlsby, S. Utili, Powder Technology, 248 (2013) 94-102.
[5] A. Wachs, L. Girolami, G. Vinay, G. Ferrer, Powder Technology, 224 (2012) 374-389.
[6] B. Smeets, T. Odenthal, J. Keresztes, S. Vanmaercke, P. Van Liedekerke, E. Tijskens, W. Saeys, H. Van Oosterwyck, H. Ramona, Comput. Methods Appl. Mech. Engrg., (2014) to appear.
[7] J.E. Andrade, K.W. Lim, C.F. Avila, I. Vlahinic, Comput. Methods Appl. Mech. Engrg., 241-244 (2012) 262-274.
[8] N.S. Weerasekara, M.S. Powell, P.W. Cleary, L.M. Tavares, M. Evertsson, R.D. Morrison, J. Quist, R.M. Carvalho, Powder Technology, 248 (2013) 3-24.

Resume

Dr. Tomasz Koziara is a Lecturer in computational/theoretical solid mechanics at Durham University's School of Engineering and Computing Sciences. He completed his Masters degree in Computational Mechanics (and Civil Engineering) at Cracow University of Technology in Poland. Subsequently, he moved to industry and for several years worked as a software engineer implementing Finite Element Method solvers for civil engineering. This was followed by doctoral studies at the University of Glasgow focused on development of multibody contact algorithms [A,B]. His PhD thesis titled "Aspects of Computational Contact Dynamics" received the ECCOMAS award as one of two best European PhD theses in 2008 on computational methods in applied sciences and engineering. Recently his work has focused on a High Performance Computing (HPC) implementation of SOLFEC, an open-source implicit multibody contact/impact dynamics code [C]. This research is motivated by cooperation with industry, in the development of an efficient implicit multibody approach for the dynamic analysis of nuclear graphite cores.

[A]. Koziara, T. and Bićanić, N., Semismooth Newton method for frictional contact between pseudo-rigid bodies, *Computer Methods in Applied Mechanics and Eng* (2008), 2763-2777.
[B]. Koziara, T. and Bićanić, N., Simple and efficient integration of rigid rotations suitable for constraint solvers, *Int. Journal for Numerical Methods in Engineering* (2009), 1073-1092.
[C]. Koziara, T. and Bićanić, N., A distributed memory parallel multibody Contact Dynamics code, *International Journal for Numerical Methods in Engineering* (2011), 437-456.