Patent Issued for Method, Apparatus and Computer Program for Multiple Time Stepping Simulation of a Thermodynamic System Using Shadow Hamiltonians

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By a News Reporter-Staff News Editor at Journal of Engineering -- According to news reporting originating from Alexandria, Virginia, by VerticalNews journalists, a patent by the inventors Akhmatskaya, Elena Vitalievna (Chalfont St. Peter, GB); Reich, Sebastian (Schwielowsee, DE), filed on July 8, 2010, was published online on August 13, 2013. The assignee for this patent, patent number 8510084, is Fujitsu Limited (Kawasaki, JP). Reporters obtained the following quote from the background information supplied by the inventors: "Molecular dynamics (MD) is a useful technique for theoretical investigation of molecular systems such as biomolecular systems and other macromolecular systems. A primary limitation in the application of MD to the study of complex processes involving macromolecules, e.g. biomolecules, is the small time step size of conventional MD. Whereas the latter is typically measured in femtoseconds, some dynamical processes of interest happen in microseconds and longer time scales. Bridging the time scale gap between simulations and the phenomena of interest has been an area of active research for more than a decade. A variety of techniques have been introduced in order to increase the time step in molecular dynamics simulations. "One common approach is to constrain bond lengths using either the SHAKE (Ryckaert et al., 1977) or RATTLE (Anderson, 1983) algorithms. Although application of these methods allows for a modest (.about. a factor of 2) increase in the time step, time-dependent quantities may be affected. Additionally, the constraint methods have not been shown to work well for bond angle degrees of freedom when applied to the case of macromolecules (van Gunsteren et al., 1982). "An additional complication is that biological and some other complex systems are multi-scale in nature. For example, the dynamics of proteins contain motions over different time scales, from atomic vibrations in the order of femtoseconds to collective motions at millisecond scales. FIG. 1 depicts the dynamics of molecules such as protein molecules, to illustrate the variation in time scales. "Traditional time stepping integrators (e.g. Verlet) commonly used in molecular

dynamics (MD) are not able to address this time scale problem. A typical time-step for these methods is 1 femtosecond. This makes atomistic simulation of biomolecules computationally extremely expensive. Multi-scale numerical methods, in which the presence of fast scales does not affect the time integration of slow scales, are urgently needed for efficient simulation of large biomolecular systems. Such approaches, in theory, can essentially enhance performance of molecular simulation since the most computationally expensive long-range electrostatic interactions contribute to the dynamics on relatively long time scales (compared with internal vibrations) and thus ideally do not need to be calculated frequently. Also, such approaches enhance the data locality which makes them better suited for implementation on parallel computers than traditional MD schemes. "One approach is to separate the dynamics into fast, uninteresting modes, and slow, functionally relevant modes and perform MD in the reduced space. Among the most popular approaches to find reduced dynamical spaces for biomolecules are normal mode analysis (NMA) (Levitt et al., 1985) and principal component analysis (PCA) (Balsera et al., 1996). Those methods have been combined with various computational schemes (e.g. LIN (Zhang et al., 1993), ACM (Zhang et al., 2003), LLMOD (Kolossvary et al., 2001), SMD (Space et al., 1993), NML (Sweet et al., 2008)) to yield simulation techniques which, in fact, have not succeeded in either providing the desired accuracy or in achieving substantial computational speed-up (Sweet et al., 2008) for atomistic simulation of macromolecules.