Teaching Materials Science Using a Client-Side Force-Directed Graph Framework

Georgios Varnavides*
Department of Materials Science and Engineering
Massachusetts Institute of Technology, Cambridge, MA 02139, USA

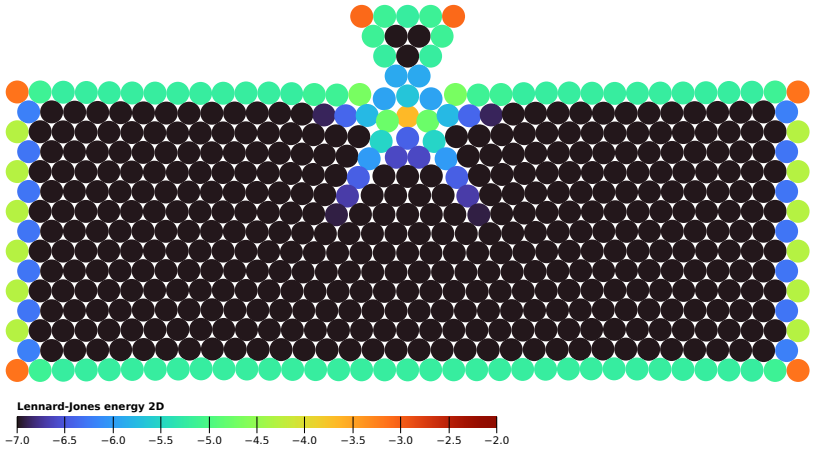

Figure 1: Snapshot of an indentation experiment simulation using the developed framework. Triangular indentation probe is made up of rigid particles moving at a constant velocity. The thin 'beam' is made up of hexagonally-closed packed particles interacting with each other and the indentation probe using a normalized Lennard-Jones interatomic potential. The beam's left and right edges are held fixed. All particles are coloured according to their Lennard-Jones potential. Lines of higher energy concentration signal the onset of dislocations forming, allowing the beam to deform plastically.

Abstract

Duis autem vel eum iriure dolor in hendrerit in vulputate velit esse molestie consequat, vel illum dolore eu feugiat nulla facilisis at vero eros et accumsan et iusto odio dignissim qui blandit praesent luptatum zzril delenit augue duis dolore te feugait nulla facilisi. Lorem ipsum dolor sit amet, consectetuer adipiscing elit, sed diam nonummy nibh euismod tincidunt ut laoreet dolore magna aliquam erat volutpat. Ut wisi enim ad minim veniam, quis nostrud exerci tation ullamcorper suscipit lobortis nisl ut aliquip ex ea commodo consequat. Duis autem vel eum iriure dolor in hendrerit in vulputate velit esse molestie consequat, vel illum dolore eu feugiat nulla facilisis at vero eros et accumsan et iusto odio dignissim qui blandit praesent luptatum zzril delenit augue duis dolore te feugait nulla facilisi.

Index Terms: Force-directed graphs — Visualization systems and education tools;

1 Introduction

Force-directed graph layouts describe a broad class of algorithms which attempt to visualize the relationships between nodes in undirected graphs and hierarchical trees, via means of a physical simulation [3, 8, 10]. Such graph layouts have recently enjoyed increased popularity in the domain of information visualization, given the rise of interactive visualizations and advancements in just-in-time compilers for Javascript [4, 5]. Further, the level of maturity, and integration with web-standards, of various Document Object Model (DOM) manipulation libraries, such as D3.js [1], suggest that physical simulations, even beyond the scope of typical graph layouts, can be carried out dynamically and interactively on the client-side. Here, we explore the merits of this idea in the context of undergraduate education. In particular, we extend one such popular force-directed graph implementation, namely D3.js's *d3-force* module, to perform energy-conserving velocity Verlet integration and implement new forces commonly used in molecular dynamics simulations of condensed matter systems. We then use this module to develop an interactive narrative [7], illustrating various core concepts in materials science, such as the formation of dislocations during plastic deformation (Fig. 1).

*e-mail: gvarnavi@mit.edu

2 Related Work

Despite using physical simulations at their core, force-directed graph algorithms solve a specific problem with notably different objectives and priorities than molecular dynamics. For example, contrary to molecular dynamics simulations, accuracy is often not the primary concern and instead visual clarity and stability are prioritized during design decisions [6]. As such, the work presented here is best compared against both force-directed graph algorithms, but also client-side dynamic physics engines.

2.1 Force-Directed Graph Layout Frameworks

While there exist multiple force-directed graph layout implementations, here we focus on some well-suited for dynamic and interactive exploration of graph data.

One popular such framework is included as a core module in D3.js, aptly called *d3-force*. It implements a simplified velocity Verlet numerical integrator, with a unit mass and time-step (see Sect. 3),

converging to a stable configuration using 'temperature' annealing. The module presented here is very closely related to *d3-force*, and in-fact builds on *d3-force* source code to address two short-comings (in the context of molecular dynamics):

1. Link constraints in *d3-force* use iterative-relaxation (effectively peeking-ahead at node's anticipated positions) to increase stability; this has consequences in energy-conservation.

2. The unit-time step assumption used in *d3-force*, followed by a simplification of the equations of motion leads to the numerical integrator accumulating error.

An alternative to *d3-force*, albeit still often used in conjunction with d3.js for displaying, is cola.js or 'WebCoLa', which instead uses constraint-based optimization techniques to converge to a local optimum. Such constraint optimization often leads to higher quality layouts, with increased stability. However, as it is solving an optimization problem – as opposed to solving some equations of motion – it is less applicable to molecular dynamics simulations.

2.2 Client-Side Dynamic Physics Engines

Perhaps a more natural comparison to the work presented here on dynamic molecular dynamics simulations are client-side Javascript physics engines. Among these, *matter.js* and *planck.js* are most closely-related as they also use a Verlet numerical integrator to solve the equations of motion [2, 9]. A great deal of attention has been spent in making *matter.js* and *planck.js* work with client-side applications in mind with the resulting simulations being seamlessly interactive as-well as performant. In contrast to d3.js, it is built on top of HTML5 and thus works by manipulating the canvas – as opposed to scalable vector graphics.

3 Methods

Molecular dynamics simulations numerically integrate Newton's equations of motions for an ensemble of forces acting on particles, by taking small finite time-steps. At each set of particle positions, the forces acting on the particles as-well as their velocities are used to predict the new particle positions a finite time step away. An important family of numerical integrators used in molecular dynamics simulations were re-discovered by L. Verlet in 1967 [11].

3.1 Position Verlet Integration

Starting from Newton's equations of motion

$$\vec{F} = m\,a\left(\vec{x}(t)\right) = m\,\ddot{\vec{x}}(t), \tag{1}$$

where F and m are the force and mass experienced by a particular particle, and $a\left(\vec{x}(t)\right)$ is the instantaneous acceleration of particle particle at position $\vec{x}(t)$ at time t. The second-order differential equation can be solved with appropriate initial conditions $\vec{x}(t_0) = \vec{x}_0$ and $\dot{\vec{x}}(t_0) = \vec{v}_0$ at time $t_n = t_0 + n\Delta t$ using the recurrence relation:

$$\begin{aligned}
\vec{x}_1 &= \vec{x}_0 + \vec{v}_0\Delta t + a\left(\vec{x}_0\right)\Delta t^2 + \mathcal{O}(\Delta t^4) \\
\vec{x}_{n+1} &= 2\vec{x}_n - \vec{x}_{n-1} + a\left(\vec{x}_n\right)\Delta t^2 + \mathcal{O}(\Delta t^4) \\
\vec{v}_n &= \frac{1}{2\Delta t}\left(\vec{x}_{n+1} - \vec{x}_{n-1}\right) + \mathcal{O}(\Delta t^4)
\end{aligned} \tag{2}$$

While Equation 2 is fairly simple to implement and is accurate up to fourth-order in the time-step Δt, it requires one stores (at-least) three consecutive particle positions and evaluates the velocities one time-step behind the positions.

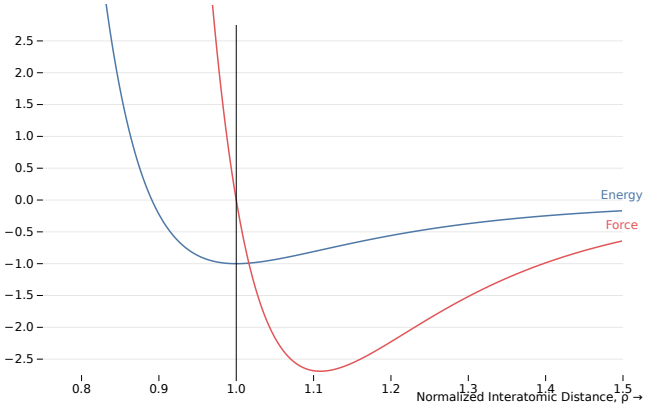

Figure 2: Normalized Lennard Jones interatomic potential (blue) and its negative gradient (red), illustrating the force experienced by a pair of particles separated a normalized distance ρ apart.

3.2 Velocity Verlet Integration

The Velocity Verlet variation addresses those short-comings by evaluating both the positions and velocities at the same time:

$$\begin{aligned}
\vec{x}_{n+1} &= \vec{x}_n + \vec{v}_n\Delta t + \frac{a\left(\vec{x}_n\right)\Delta t^2}{2} + \mathcal{O}(\Delta t^3) \\
\vec{v}_{n+1} &= \vec{v}_n + \frac{\Delta t}{2}\left(a\left(\vec{x}_{n+1}\right) + a\left(\vec{x}_n\right)\right) + \mathcal{O}(\Delta t^3)
\end{aligned} \tag{3}$$

In particular, we evaluate Equation 3 in three steps:

$$\begin{aligned}
\vec{v}_{n+1/2} &= \vec{v}_n + \frac{\Delta t}{2}a\left(\vec{x}_n\right) \\
\vec{x}_{n+1} &= \vec{x}_n + \vec{v}_{n+1/2}\Delta t \\
\vec{v}_{n+1} &= \vec{v}_{n+1/2} + \frac{\Delta t}{2}a\left(\vec{x}_{n+1}\right)
\end{aligned} \tag{4}$$

3.3 Central-Body Interatomic Potentials

Central-force potentials are a family of rotationally-invariant potentials which only depend on the distance r between two particles. Here, we focus on the consequences of the Lennard-Jones potential, although we note the formalism developed here can accept general Javascript functions as interatomic potential inputs. The Lennard-Jones potential is a model for a particle's potential energy when it is separated from another particle. The model is simple – particles attract each other when they are far apart and repel when they are very near. All of the physics and its consequences derive from the shape of the potential, given by Fig. 2. When the distance is small, the potential energy decreases with increasing distance. The force is positive and repulsive because force is minus the gradient of potential energy. When the distance is large, the potential energy slope is positive and so the force is negative: the particles attract.

Mathematically, the Lennard-Jones potential is given by a linear combination of two terms: An attractive term that goes to zero as $-\frac{1}{r^6}$ as $r \to \infty$; A repulsive term that goes to infinity as $\frac{1}{r^{12}}$ as $r \to 0$

$$U_{ljp} = \frac{a}{r^{12}} + \frac{b}{r^6}, \tag{5}$$

with a and b being material-properties we could extract using experimental observations. To understand the dynamics of materials with this family of interatomic potentials however, we non-dimensionalize Equation 5 by introducing an equilibrium distance

$\rho = r/r_{min}$ and dividing the potential by the energy at that equilibrium distance:

$$\tilde{U}_{ljp} = \frac{1}{\rho^{12}} - \frac{2}{\rho^{6}}. \quad (6)$$

4 Results

4.1 Physical Origins of Surface Energy

Lorem ipsum dolor sit amet, consetetur sadipscing elitr, sed diam nonumy eirmod tempor invidunt ut labore et dolore magna aliquyam erat, sed diam voluptua. At vero eos et accusam et justo duo dolores et ea rebum. Stet clita kasd gubergren, no sea takimata sanctus est Lorem ipsum dolor sit amet. Lorem ipsum dolor sit amet, consetetur sadipscing elitr, sed diam nonumy eirmod tempor invidunt ut labore et dolore magna aliquyam erat, sed diam voluptua. At vero eos et accusam et justo duo dolores et ea rebum. Stet clita kasd gubergren, no sea takimata sanctus est Lorem ipsum dolor sit amet. Lorem ipsum dolor sit amet, consetetur sadipscing elitr, sed diam nonumy eirmod tempor invidunt ut labore et dolore magna aliquyam erat, sed diam voluptua. At vero eos et accusam et justo duo dolores et ea rebum.

5 Discussion

Lorem ipsum dolor sit amet, consetetur sadipscing elitr, sed diam nonumy eirmod tempor invidunt ut labore et dolore magna aliquyam erat, sed diam voluptua. At vero eos et accusam et justo duo dolores et ea rebum. Stet clita kasd gubergren, no sea takimata sanctus est Lorem ipsum dolor sit amet. Lorem ipsum dolor sit amet, consetetur sadipscing elitr, sed diam nonumy eirmod tempor invidunt ut labore et dolore magna aliquyam erat, sed diam voluptua. At vero eos et accusam et justo duo dolores et ea rebum. Stet clita kasd gubergren, no sea takimata sanctus est Lorem ipsum dolor sit amet. Lorem ipsum dolor sit amet, consetetur sadipscing elitr, sed diam nonumy eirmod tempor invidunt ut labore et dolore magna aliquyam erat, sed diam voluptua. At vero eos et accusam et justo duo dolores et ea rebum.

6 Future Work

Lorem ipsum dolor sit amet, consetetur sadipscing elitr, sed diam nonumy eirmod tempor invidunt ut labore et dolore magna aliquyam erat, sed diam voluptua. At vero eos et accusam et justo duo dolores et ea rebum. Stet clita kasd gubergren, no sea takimata sanctus est Lorem ipsum dolor sit amet. Lorem ipsum dolor sit amet, consetetur sadipscing elitr, sed diam nonumy eirmod tempor invidunt ut labore et dolore magna aliquyam erat, sed diam voluptua. At vero eos et accusam et justo duo dolores et ea rebum. Stet clita kasd gubergren, no sea takimata sanctus est Lorem ipsum dolor sit amet. Lorem ipsum dolor sit amet, consetetur sadipscing elitr, sed diam nonumy eirmod tempor invidunt ut labore et dolore magna aliquyam erat, sed diam voluptua. At vero eos et accusam et justo duo dolores et ea rebum.

Acknowledgments

The authors acknowledgement Craig Carter and Amina Matt of the Massachusetts Institute of Technology for fruitful discussions and the initial authoring and editing of the materials-specific simulations.

References

[1] M. Bostock, V. Ogievetsky, and J. Heer. D3: Data-driven documents. *IEEE Trans. Visualization & Comp. Graphics (Proc. InfoVis)*, 2011.

[2] L. Brummitt. Matter.js: a 2d rigid body physics engine for the web. `https://github.com/liabru/matter-js`, 2014.

[3] P. Eades. A heuristic for graph drawing. *Congressus Numerantium*, vol.42:149–160, 1984.

[4] A. Gal, B. Eich, M. Shaver, D. Anderson, D. Mandelin, M. R. Haghighat, B. Kaplan, G. Hoare, B. Zbarsky, J. Orendorff, J. Ruderman, E. W. Smith, R. Reitmaier, M. Bebenita, M. Chang, and M. Franz. Trace-based just-in-time type specialization for dynamic languages. *SIGPLAN Not.*, 44(6):465–478, June 2009. doi: 10.1145/1543135.1542528

[5] B. Hackett and S.-y. Guo. Fast and precise hybrid type inference for javascript. *SIGPLAN Not.*, 47(6):239–250, June 2012. doi: 10.1145/2345156.2254094

[6] T. Jakobsen. Advanced character physics. In *IN PROCEEDINGS OF THE GAME DEVELOPERS CONFERENCE 2001*, p. 19, 2001.

[7] D. E. Knuth. Literate Programming. *The Computer Journal*, 27(2):97–111, 01 1984. doi: 10.1093/comjnl/27.2.97

[8] S. G. Kobourov. Spring Embedders and Force Directed Graph Drawing Algorithms. *arXiv e-prints*, p. arXiv:1201.3011, Jan. 2012.

[9] A. Shakiba. Matter.js: a 2d rigid body physics engine for the web. `https://github.com/shakiba/planck.js`, 2017.

[10] W. T. Tutte. How to draw a graph. *Proceedings of the London Mathematical Society*, s3-13(1):743–767, 1963. doi: 10.1112/plms/s3-13.1.743

[11] L. Verlet. Computer "experiments" on classical fluids. i. thermodynamical properties of lennard-jones molecules. *Phys. Rev.*, 159:98–103, Jul 1967. doi: 10.1103/PhysRev.159.98