

# 18.337 Project: A Random Walk with Julia

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## 1 Introduction

As the title suggests, this document is a review of a newcomer's journey into the world of Julia. In particular, the newcomer is user rather than a developer. Two different applications of Julia are reviewed, and the issues encountered along the way are discussed.

## 2 Part 1

The characteristic vibrational modes of a physical system are determined by the potential energy term of the system's Hamiltonian. These vibrations are of interest because of their properties govern thermal transport in semiconductors. The second order derivatives of the potential energy with respect to displacements about the equilibrium position of the atoms, colloquially referred to as the second order force constants, is a positive definite block-diagonal Hessian matrix. We start with the simple one-dimensional mass-spring configuration, as shown in Fig. 1. Here,  $u_n$  is the displacement from equilibrium of the  $n$ th atom with mass  $m$  and  $U_n$  is the displacement from equilibrium of the  $n$ th of atom with mass  $M$ . The equations of motion of a linear diatomic chain considering only nearest neighbour interactions ( $K_1$

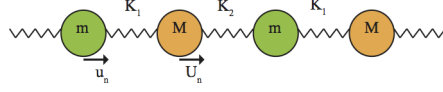


Figure 1: Diagram of a linear diatomic chain of atoms.

and  $K_2$  are the respective spring constants in accordance with Hooke's Law)

$$M \frac{\partial^2 U_n}{\partial t^2} = -K_1(U_n - u_n) - K_2(U_n - u_{n-1}) \quad (1)$$

$$m \frac{\partial^2 u_n}{\partial t^2} = -K_1(u_n - U_n) - K_2(u_n - U_{n+1}) \quad (2)$$

The coupled ordinary differential equations can be represented as a matrix equation,  $KM^{-1}U = 0$ , assuming a plane wave solution for atomic displacement. The square root of the eigenvalues of  $KM^{-1}$  are the harmonic frequencies of the characteristic vibrational modes. For this one-dimensional case with the masses are set to unity and  $M$  is the identity matrix, the vibrational properties are determined by the stiffness matrix

$$K_{ordered} = \begin{bmatrix} 2 & -1 & 0 & \cdots & -1 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ -1 & 0 & \cdots & -1 & 2 \end{bmatrix}. \quad (3)$$

For a perfect systems, the spring constants are equal between atoms. Understanding the effects of disorder (i.e.: point defects, isotopes, alloying elements or amorphous phases) is critical in order to be able to engineer materials with specific thermal transport properties. Typically, disorder is treated as a perturbation of the perfect system [1, 2, 3, 4, 5]. The validity of this assumption is questionable and does not necessarily hold for all cases [6]. Disorder can manifest through the spring matrix or the mass matrix. In this study, disorder is controlled through the manipulation of the spring constants. Localized disorder, such as a point defect, is introduced by tweaking the spring constants of a select few atoms. For example, the parameter  $p$  tunes the spring constants attached to the first atom

$$K_{defect} = \begin{bmatrix} 2p & -1p & 0 & \cdots & -1p \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ -1 & 0 & \cdots & -1 & 2 \end{bmatrix}. \quad (4)$$

Delocalized disorder, such as amorphous or glassy systems, manifests in terms of much longer range interactions. Here, this interaction is introduced through an off-diagonal element parameter  $p$

$$K_{lr} = \begin{bmatrix} 2+p & -1 & 0 & \cdots & -p & 0 & \cdots & -1 \\ -1 & 2+p & -1 & \cdots & 0 & -p & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & & & \ddots & \vdots \\ -p & \cdots & -1 & 2+p & -1 & \cdots & \cdots & 0 \\ 0 & -p & \cdots & -1 & 2+p & -1 & \cdots & 0 \\ \vdots & & \ddots & & \ddots & \ddots & \ddots & \vdots \\ -1 & 0 & \cdots & -p & \cdots & \cdots & -1 & 2+p \end{bmatrix}. \quad (5)$$

This type of disorder is very much analogous to the coupling between graphs discussed by Radicchi and Arenas [7]. Their work demonstrated an abrupt transition in the behavior of the Fiedler eigenvalue,  $\Lambda_2$ , of interconnected graphs as a function of the strength of the coupling,  $p$ , between graphs [7]

$$\begin{bmatrix} \mathcal{L}_A + p\mathbb{1} & -p\mathbb{1} \\ -p\mathbb{1} & \mathcal{L}_B + p\mathbb{1} \end{bmatrix} \quad (6)$$

By tuning  $p$  for the single defect and delocalized cases, its effect on the Fiedler eigenvalue can be examined. Naturally, Julia's implementation is succinct. Although these matrices are sufficiently sparse, the eigenvalues obtained from the `eigs` call deviated from those obtained with `eig` as shown in the appendix.<sup>1</sup>

Good agreement between the `eig` results for the perfect and long range case obtained from Julia when compared against the equivalent MATLAB implementation were found (see Fig. 2). Note that the single defect case differed considerably, which is likely the consequence of how each language handles numerical precision.

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<sup>1</sup>There is ongoing discussion about the future of `eigs` with the developers of Julia. See Issues [1573](#) and [2956](#) for example.

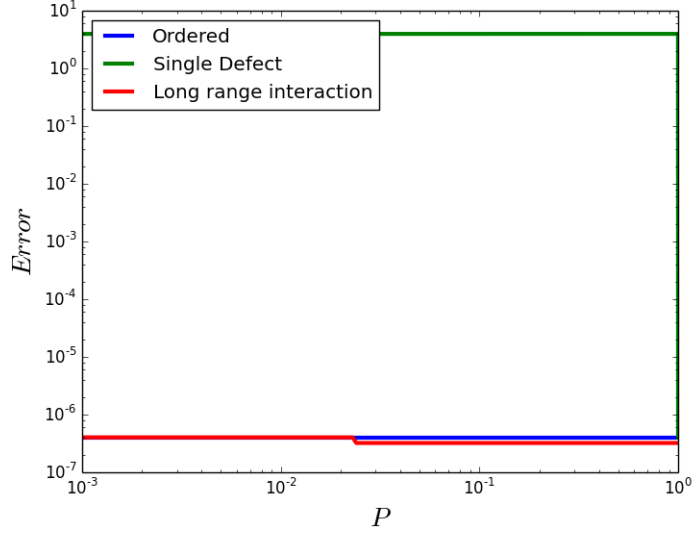


Figure 2: Absolute difference between Fiedler eigenvalues obtained from Julia and MATLAB using `eig`.

```

function p_feidler(n,pp)
    lam = @parallel (hcat) for p =1:length(pp)
        #construct matrix
        k=2*eye(n)-circshift(eye(n),1)
            -circshift(eye(n),-1)
        #insert off-diagonal elements
        #subtract pI from diagonal
        pr=pp[p]
        k=k-pr.*circshift(eye(n),-int(n/2))
            +pr.*eye(n)
        #take eig
        real(eig(k)[1][2])
    end
    return pp,lam
end

```

In Fig. 3, the results of a 50 atom case are presented.<sup>2</sup> For single defects, the eigenvalue converges to the perfect case, while for long range disorder, a

<sup>2</sup>While the absolute values of the eigenvalues changed for larger matrices, the trends did not.

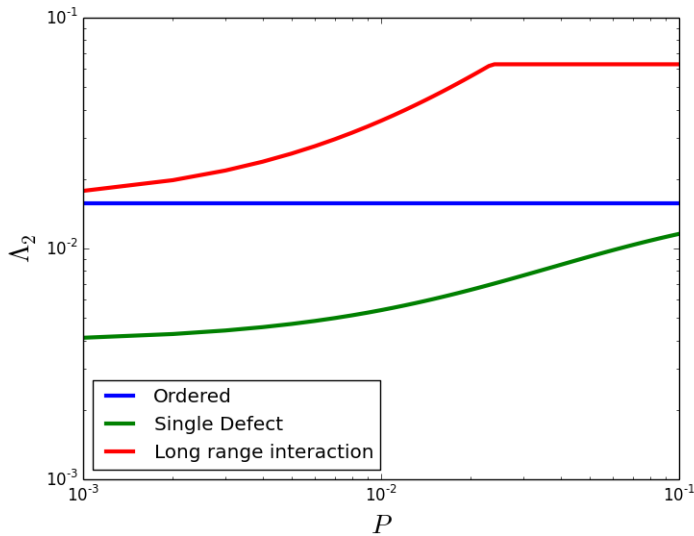


Figure 3: A sample result from a 1D chain.

discontinuity is observed like in the work of Radicchi and Arenas [7].

Trivial parallelism is used via the `@parallel` macro, since disorder is an independent parameter. A comparison of the serial and parallel scalings as function of matrix size is presented in Fig. 4.

This work is currently being extended to study real materials, specifically bulk silicon with disorder being determined through the controlling the concentration of an alloying element like germanium. The objective is to express the disorder parameter in terms of material properties.

### 3 Part 2

As an exercise in the history of science, the user obtained [citation data from the American Physical Society](#), which contains all citation pairs from within the APS journal family from 1893 to 2009. This information can be represented as a directed graph, where the papers are the nodes and the citations are the edges. This effort was inspired by [Citerank](#), which is a pagerank application to scientific articles, and [Eigenfactor](#), which studies the connectedness at the journal to journal level.

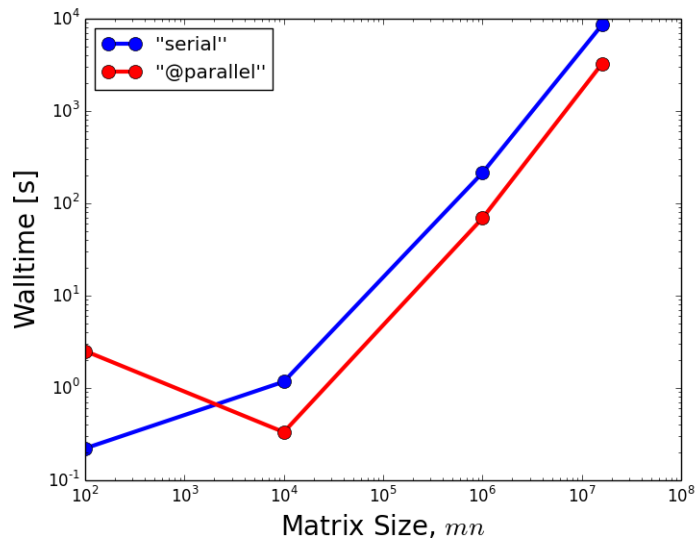


Figure 4: A comparison of the wall time as a function of matrix. As expected, the parallel approach is nearly four times faster than the serial version. The speed up is independent for large matrix sizes.

The user attempted to develop a parallel version of a breadth first search, but the [Graphs.jl package](#) developed by Dahua Lin proved to be a much better choice.

```
function papertree(doi_to, doi_from)

    g=as_deserialized("graph.txt")
    citing=readcsv("unique.csv")

    c=Dict{ASCIIString,Int}()
    for i=1:length(citing)
        c[citing[i]]=i
    end

    #set all distances to 1, hack to use dijkstra's
    dists=ones(num_edges(g))
    r = dijkstra_shortest_paths(g, dists, c[doi_from])

    l=c[doi_to]
    pt={}

    for d=1:r.dists[c[doi_to]]
        l=r.parents[l]
        push!(pt,string("http://link.aps.org/doi/",citing[l],"\n"))
    end

    return pt

end
```

As part of randomly walking with Julia, the user explored the current status of web-related packages. While the user has no experience with web development, the current breadth of Julia is exciting because it offers the opportunity to venture outside one's skill set without having to switch to a different language. In the code snippet below, a simple HTTP service is presented. The user provides the digital object identifier (DOI) of an APS journal article in the URL and the response returns the trail of papers, if one exists, to the 1964 paper by Peter Higgs.

```
using HttpServer
require("nobel.jl")

http = HttpHandler() do req::Request, res::Response
    m = match(r"^/doi/(.*)", req.resource)
```

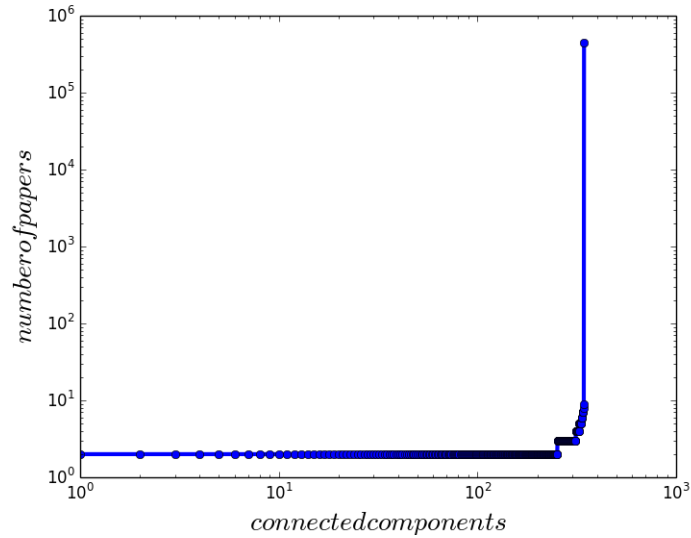


Figure 5: The number of papers in each subgraph.

```

if m == nothing return Response(404) end
p=papertree(string(m.captures[1]),"10.1103/PhysRevLett.13.508")
println(m.captures[1])
return Response(string(p))
end

http.events["error"] = (client, err)-> println(err)
http.events["listen"] = (port) -> println("Listening on $port...")

server = Server(http)
run(server, 8000)

```

Currently, the graph and the unique list of papers are read in with each call of `papertree`. For a real-time web application, this graph should be converted to a database. Lastly, the connected components of the citation network were examined (ignoring the direction of time and using an undirected graph). From Fig. 5, the vast majority (99.9%) of all papers in the network are connected.



## 4 Issues

Throughout this project, several issues were encountered. Upon upgrading to the final version of Julia 0.2.0, the packages [GnuTLS](#) and [Homebrew](#) began to throw errors. Using Julia’s package manager to remove, upgrade and add these packages did not remove the error messages. After posting [GnuTLS issue 13](#) and [Homebrew issue 30](#) on GitHub, the issue was deemed to be the fault of the user and was resolved by deleting the .julia directory in the user’s home directory and running `Pkg.add("Homebrew")`.

Meanwhile, the user tested the new IJulia package for Sublime Text developed by Jacob Quinn. Through [testing](#), it was determined that Mac OS X requires a symlink to the ZMQ library.

Prior to discovering the `HttpServer.jl` package, the user attempted to use the `HTTP.jl`. This package was developed for an earlier version of Julia and required some maintenance. The user submitted a [pull request](#) to improve compatibility with Julia 0.2.0.

Lastly, the user gained basic familiarity with the proposed `SharedArray` [pull request](#) from Amit Murthy. The objective of this functionality is to provide a data structure that can be accessed and manipulated across all processes, accomplished through some low-level unix-system function calls. This functionality will be beneficial for the processing of large datasets.

## 5 Conclusions

Two studies using Julia are reviewed and the bugs and technical issues encountered along the way are discussed. In the first, the simplicity of harnessing trivial parallelism is shown. In the second, the `Graphs.jl` and `HttpServer.jl` packages are used to look at the citation network of the American Physical Society journal family.

The Julia experience was positive. The Julia community were responsive and helpful and did not trivialize the questions asked. The user intends to continue to learn and use Julia.

## References

- [1] Shin-ichiro Tamura. Isotope scattering of dispersive phonons in ge. *Phys. Rev. B*, 27:858–866, Jan 1983.
- [2] Maria N. Luckyanova, Jivtesh Garg, Keivan Esfarjani, Adam Jandl, Mayank T. Bulsara, Aaron J. Schmidt, Austin J. Minnich, Shuo Chen, Mildred S. Dresselhaus, Zhifeng Ren, Eugene A. Fitzgerald, and Gang Chen. Coherent phonon heat conduction in superlattices. *Science*, 338(6109):936–939, 2012.
- [3] S. P. Hepplestone and G. P. Srivastava. Phononic gaps in thin semiconductor superlattices. *Journal of Applied Physics*, 107(4):043504, 2010.
- [4] S. P. Hepplestone and G. P. Srivastava. Lattice dynamics and thermal properties of phononic semiconductors. *Phys. Rev. B*, 84:115326, Sep 2011.
- [5] Iorwerth O. Thomas and G. P. Srivastava. Thinning down of thermal conductivity in ultrashort period superlattices. *Phys. Rev. B*, 88:115207, Sep 2013.
- [6] Samuel C. Huberman, Jason M. Larkin, Alan J. H. McGaughey, and Cristina H. Amon. Disruption of superlattice phonons by interfacial mixing. *Phys. Rev. B*, 88:155311, Oct 2013.
- [7] Filippo Radicchi and Alex Arenas. Abrupt transition in the structural formation of interconnected networks. *Nature Physics*, 2013.

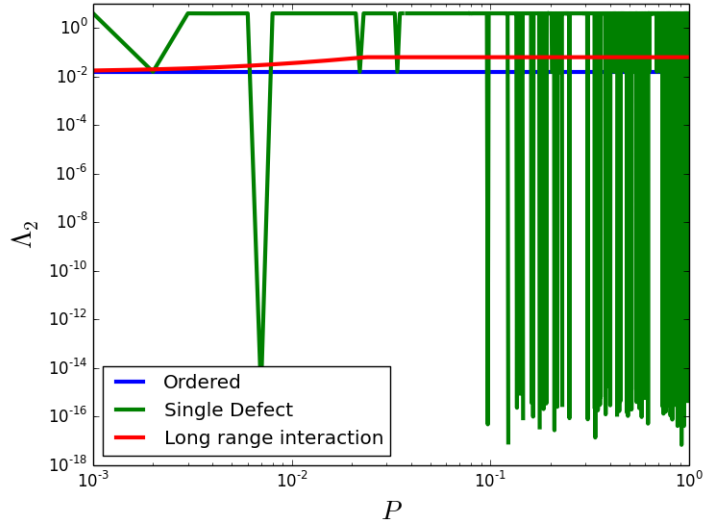


Figure 6: Fiedler eigenvalues obtained using `eigs`.

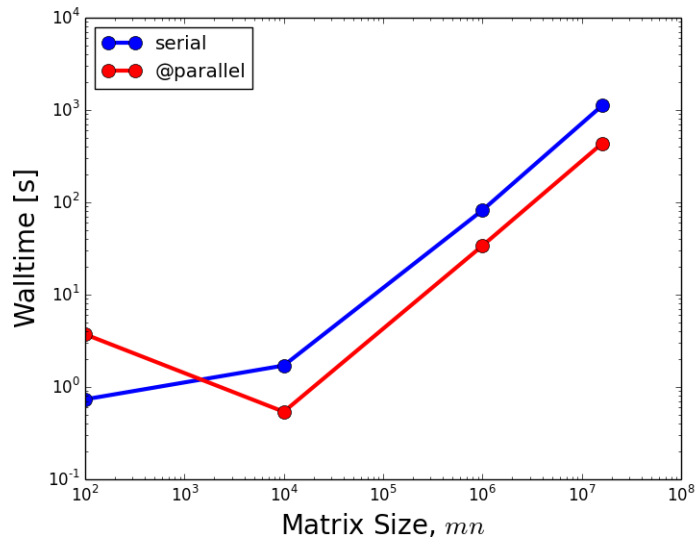


Figure 7: A comparison of the wall time as a function of matrix using `eigs`.