

**Fall 2019**

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## **Molecular-Scale Insight into Novel Energy-Storage Materials Using Dynamics Simulations Employing Polarizable Force Fields**

Research Highlight · Dengpan Dong and Dmitry Bedrov, Department of Materials Science and Engineering

The 2019 Nobel Prize in Chemistry was recently awarded to John B. Goodenough, M. Stanley Whittingham, and Akira Yoshino for their pioneering studies in the development of lithium-ion batteries (LiBs), one of the most common energy storage systems. LiBs are used to power common electronic devices such as phones and laptops, for large-scale grid energy storage, and in electric vehicles, to name just a few of the many applications of this technology. The ceaselessly increasing demand for clean and renewable energy is motivating researchers to look for higher energy density as well as for safer LiBs. The key to achieve these goals is to find electrolytes with high lithium-ion conductivity along with a wide electrochemical stability window. Furthermore, during charging/discharging the formation of solid-electrolytes interphase (SEI) and cathode-electrolytes interphase (CEI) layers take place; this protects electrolytes from further decomposition but creates additional resistance for Li ion transport.

Modern characterization techniques can provide nano-scale visualizations and an understanding of the processes occurring inside electrodes and electrolytes as well as at their interfaces. However, an understanding of physico-chemical processes at molecular or atomistic level is often needed. Molecular dynamics (MD) simulation is one of the tools that can be used to study the structure, dynamics, and mechanical properties of LiB components. In addition to the efforts in the LiB technologies, advances in other alternative energy storage and conversion systems, including alkaline fuel cells (AFCs) and super-capacitors, also rely on our ability to obtain physicochemical insights at molecular level in order to enable the efficient design of these new, novel materials.

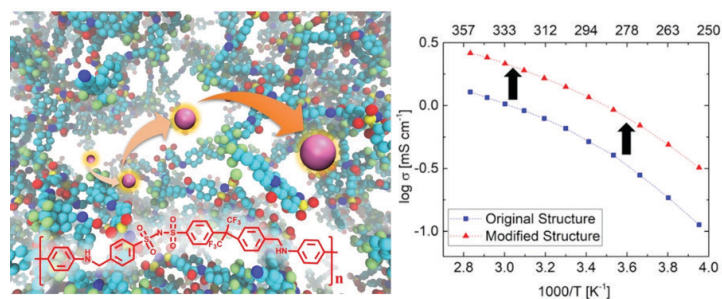
The Multiscale Simulation Group of Prof. Bedrov at the Materials Science and Engineering Department

(<https://my.eng.utah.edu/~bedrov/>) is one of the hubs for the development of molecular simulation tools including the development of the Atomistic Polarizable Potentials for Liquids, Electrolytes and Polymers (APPLE&P) force field. As has been demonstrated over the last decade, the inclusion of induced polarization in ionic systems is crucial in order to accurately capture local coordination of ions and their transport in MD simulations. Simulations that do not include induced polarization often underestimate ion dynamics by an order of magnitude compared to experiments. Some studies employ unphysical empirical adjustments to force field parameters, which may result in improved agreement with experimental results, but do not provide any insight. On the other hand, simulations using polarizable models provide an accurate description of transport and thermodynamic properties and hence can be reliably used for a virtual design of novel materials. Below we illustrate several projects that employ polarizable MD to study energy storage and conversion systems.

### **Design of Novel Electrolytes for LiBs**

In joint studies with experimental groups from the Army Research Lab (Maryland, US) and the Münster Electrochemical Energy Technology Center (Münster, Germany), a number of novel polymer-based electrolytes, including polysulfonimide-based single ion conductor gels, water-in-salt electrolytes (WiSEs), and polyrotaxanes (PRs) have been investigated for application in new LiB technologies. All these electrolytes are much safer compared to standard organic liquid electrolytes currently employed. These new electrolytes also potentially provide additional benefits such as the suppression of the growth of Li metal dendrites at electrode surfaces (which reduce battery capacitance and eventually lead to battery failure) and the possibility

of making flexible, non-leaking batteries. The transport of  $\text{Li}^+$  ions between the electrodes is strongly correlated with the chemical structure of functional groups comprising the polymer chains along with the spatial distribution of nano-sized, self-assembled clusters of those functional groups. In single-ion gel electrolytes, molecular simulations allowed us to identify specific segments/chemical groups that were trapping  $\text{Li}^+$ , therefore hindering its diffusion through solvent domains and limiting its long-distance transport. Using the information provided by the simulations, synthetic chemists modified the polymer structures to eliminate the  $\text{Li}^+$  trapping sites. Figure 1 illustrates that a three-fold increase in  $\text{Li}^+$  conductivity was achieved with a battery cell using the modified polymer structure, without any detrimental effects being observed. Using the modified polymer, a single-ion gel electrolyte with the highest reported conductivity (for this class of materials) of 0.2 mS/cm at room temperature was designed.



**Figure 1.** Novel single ion conductor polymer gel synthesized based on physical insight into Li-polymer/solvent correlations at molecular scale obtained from MD simulations.

Low  $\text{Li}^+$  transference numbers (the fraction of ionic conductivity due to  $\text{Li}^+$  transport) and the leakage from the cell are two major challenges tempering the application of novel WiSE electrolytes. Turning WiSEs into gel-type electrolyte with the addition of poly(methyl methacrylate) polymer provides a potential solution to these issues. Our MD simulations allowed for an understanding of how the polymer chains are distributed in the WiSEs and provided the desired mechanical stability of the gel while having minor effect on  $\text{Li}^+$  transport.

In the polyoxane-based electrolytes, i.e., all-solid polymer electrolytes comprised of macromolecular assemblies, our MD simulations demonstrated that it is possible to decouple the optimization of  $\text{Li}^+$  conduction from the mechanical properties of electrolyte. Short side chains grafted outside of supramolecular tubes maximize the inter-chain hopping of  $\text{Li}^+$ , therefore facilitating  $\text{Li}^+$  transport, while linear polymer chains threading ring-like molecules provide molecular weaving that controls the mechanical properties.

## Mechanisms of Interphase Formation in LiBs

Despite the endeavors to develop high-voltage electrode materials to achieve improved energy density, battery life still suffers from degradation of electrolytes and electrodes. Typically, a thin layer near the surface of anode (the solid electrolyte interphase, SEI) is formed from the products of the electrolyte redox decomposition. This layer passivates the active sites on the anode, suppressing the growth of  $\text{Li}^+$  dendrites, but at the same time, creates an additional resistance for  $\text{Li}^+$  transport between electrode and electrolyte. Therefore, the design of SEIs is an active research field, with researchers working to identify additives or processing conditions that would produce SEIs that suppress dendrite growth while still having a low free energy barrier for  $\text{Li}^+$  transport. However, the understanding of the mechanisms of SEI formation is limited due to the lack of physical insights at molecular level. MD simulations combined with Monte Carlo processes to insert or remove redox reaction products paved the path for the simulation of SEI formation. Using these methods, our simulations indicate that the  $\text{LiF}$  and  $\text{Li}_2\text{CO}_3$  polycrystalline structures form the inner SEI layer, while the outer SEI layer is primarily comprised of longer organic oligomers (e.g. dilithium dicarbonates).

While the SEI formation on the anode has received significant attention from researchers, the formation and stability of CEI (the passivation layer formed on the cathode due to oxidation of electrolyte) has not been as widely studied. Recent studies revealed that a stable CEI is indispensable for high-voltage battery systems. In our group, we are developing novel approaches to simulate the cathode and CEI with enabled charge fluctuation between an ion and the nearest neighbors.

## Hydroxide Transport and Functional-group Degradation Mechanism in AFCs

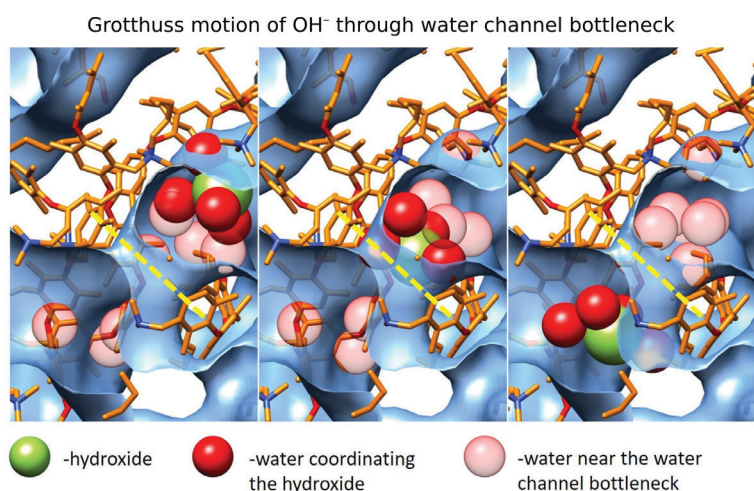
Alkaline fuel cells (AFCs) are another class of emerging energy-conversion systems for alternative energy resources. In AFCs, the charge carrier between the electrodes is the hydroxide ( $\text{OH}^-$ ) anion (unlike protons in a typical proton exchange fuel cells). The design of polymer membranes for AFCs is challenging, as the membrane must be good at facilitating charge transport while being chemically stable in an alkaline environment. In collaboration with experimental groups, we have investigated promising candidate membranes comprised of poly(p-phenylene oxide) or polysulfone backbone chains functionalized with quaternary ammonium cations.

In a hydrated membrane, there are two possible mechanisms for  $\text{OH}^-$  transport:

(1) the Grotthuss hopping mechanism: an H atom from a water molecule is transferred to OH<sup>-</sup> with the water donating the H becoming OH<sup>-</sup>

(2) vehicular motion: diffusion of OH<sup>-</sup> without O–H bond breaking/formation.

There is an ongoing debate regarding which of these mechanisms plays a substantial role in AFC membranes. Using combined reactive and non-reactive force fields, we have demonstrated the significant role of the Grotthuss motion in facilitating the transport of OH<sup>-</sup> through the sub-nanometer water channels in AFCs membranes (illustrated in Figure 2) and the ability to design polymer function groups that enhance electrochemical stability.



**Figure 2.** Illustration of the Grotthuss mechanism facilitating transport of OH<sup>-</sup> through a bottleneck in the sub-nanometer water channels.

## CHPC Contribution

The simulation studies mentioned in this article were conducted primarily using CHPC’s computational resources. Most of the studies require the generation of extremely long simulation trajectories, which would take multiple years on a single node or CPU. Therefore, the ability to access massively parallel architectures along with generous allocations of computer time were key to enable molecular simulations of these complex systems. The regular maintenance of compilers and computer nodes ensures the reliability and efficiency of our simulations.

## References

- [1] Bedrov, D., Piquemal, J. P., Borodin, O., MacKerell Jr, A. D., Roux, B., & Schröder, C. (2019). Molecular dynamics simulations of ionic liquids and electrolytes using polarizable force fields. *Chemical Reviews*, 119(13), 7940–7995.
- [2] Imholt, L., Dong, D., Bedrov, D., Cekic-Laskovic, I., Winter, M., & Brunklaus, G. (2018). Supramolecular self-assembly of methylated

rotaxanes for solid polymer electrolyte application. *ACS Macro Letters*, 7(7), 881–885.

[3] Dong, D., Zhang, W., van Duin, A. C., & Bedrov, D. (2018). Grotthuss versus vehicular transport of hydroxide in anion-exchange membranes: Insight from combined reactive and nonreactive molecular simulations. *The Journal of Physical Chemistry Letters*, 9(4), 825–829.

[4] Zhang, W., Dong, D., Bedrov, D., & van Duin, A. C. (2019). Hydroxide transport and chemical degradation in anion exchange membranes: A combined reactive and non-reactive molecular simulation study. *Journal of Materials Chemistry A*, 7(10), 5442–5452.

## Upcoming Changes to Lonepeak

News and Updates · Brian Haymore and Anita Orendt

Over the next few months, users will see a change in the nodes available on lonepeak. Thanks to donations of hardware from both Cancer Computer ([cancercomputer.com](http://cancercomputer.com)) and the University of Utah Hospital, we will be adding 192 nodes. Cancer Computer is a Canadian charity that partners with a number of institutions in Canada and the US to provide cancer research with computing power. The University of Utah Hospital provides CHPC with access to hardware that is out of warranty and therefore being retired due to the critical role it serves in support of patient care. Such hardware, however, is still suitable for use in research computing.

While these nodes are not new, they are newer than the current nodes on lonepeak (and the nodes on ember). This replacement will provide consistency among the lonepeak general nodes as well as a higher GB/core memory than many CHPC compute nodes. Currently, the general lonepeak nodes, outside of lp[001-016], are a mix of nodes with either 8 and 12 physical core nodes, 48 or 72 GB of memory, and varying sizes of local storage, with many of the nodes having less than 100 GB /scratch/local file systems. Each of the new nodes will have 12 physical cores, 96 GB memory, and between 0.5 and 1.2 TB local storage (for memory swap space and /scratch/local space). When the update is complete, there will be 192 of these nodes, resulting in an increase of 96 nodes over the current lonepeak. Note that there will be no change on the lp[001-016] nodes, nor with the existing lonepeak owner nodes.

The addition and replacement of nodes will occur in stages.

- *Stage 1:* Addition of 48 nodes as lp[133-180]. These were deployed in late October.
- *Stage 2:* Second addition of 48 nodes as lp[181-228]. These are scheduled to be deployed in November.
- *Stage 3:* Replacement of the existing lp[017-112], not all of which are currently functional. These will be done in batches, most likely 16 at a time. We expect to have these nodes in production before the end of 2019.

Lonepeak will continue to be run without allocation. Initially, these new nodes will be run as the current lonepeak nodes, with all users having equivalent access.

However, one requirement of the donation from Cancer Computer is that priority be given to “cancer-related research.” As a result, groups involved in research that can be considered to be cancer-related will be given priority over jobs from groups that are doing other types of research. To accomplish this, CHPC will need to establish a procedure for identifying groups involved in cancer-related research and give jobs from those groups higher priority. Groups that do not qualify for the higher priority will still be able to run, without preemption, on these nodes. The exact details of this will be announced after the deployment of the new nodes has been completed. In the long term, and also as part of the agreement, we will be exploring the ability to give access to these donated resources to users who are doing cancer-related research outside of the University of Utah and Utah State University.

## Changes to Local Scratch

News and Updates · Brian Haymore and Anita Orendt

In CHPC’s Spring 2019 newsletter, there was an article on new university-level policies governing the protection of sensitive data, discussing how CHPC is moving to employ encryption on all storage to address this policy.

While our latest group space purchases have been made with self-encrypted drives, we have not moved to purchasing self-encrypting drives on cluster nodes due to the per-node cost increase this would require (which includes not only the cost of the actual hard drive, but also for the controller needed to support a self-encrypted drive and the required license, adding several hundred dollars to the cost of a node). As a reminder, the local drives on the nodes are used to provide virtual memory (swap space), with the remainder providing the `/scratch/local` space.

As an alternative to the use of self-encrypted drives, we have been exploring the use of software encryption on the drives local to the cluster compute servers. As a result, we have determined a course of action that involves the encryption of these drives as part of the root image used to provision the node. The encryption keys are never saved, and upon reboot, the file system `/scratch/local` is re-created. As a result, there will no longer be any persistency of data on the local hard drive between reboots.

As this change does not impact the way users make use of `/scratch/local` and does not alter the current expectation of data preservation, since the data in this directory is already subject to being scrubbed according to existing CHPC policies (any data not accessed in two weeks is

scrubbed), CHPC started to deploy the disk encryption on the compute nodes in mid-October. It is now in place on the majority of the compute nodes. Once encryption has been deployed on all compute nodes, we will move to work on the interactive nodes. We note that several owner interactive nodes are using the local hard drives for purposes that require persistency; this change will not be deployed on those nodes.

As a second phase, CHPC will be implementing additional changes to the way `/scratch/local` is managed in order to make the use of this storage more predictable. Currently, jobs that use `/scratch/local` sometimes leave behind data, either because the script does not have a cleanup of this space in place, or even if it does, the cleanup is not completed due to the job failing, being preempted, or running out of time. While we do have scripts that check for the usage of `/scratch/local` on compute nodes, often new jobs are started before the cleanup of this space is performed and these subsequent jobs trying to use `/scratch/local` can fail. The introduction of node sharing complicates the process of scrubbing the `/scratch/local` space, as there is no way to definitively tie files in `/scratch/local` to a specific job when a single user has the ability to have multiple jobs on the same node.

In order to achieve this goal, three changes will be implemented:

- The permissions of the top-level `/scratch/local` will be set so that users can no longer create a directory in this space
- The job prolog (before the job starts) will make a job-level directory `/scratch/local/$USER/$SLURM_JOB_ID`, to which only the user will have access
- The job epilog will remove this job-level directory after the job has ended (regardless of the exit state)

If the directory creation via the prolog script fails, the job prolog exits as a “FAIL START,” the node is marked offline until it can be evaluated, and the job goes back into the queue (with the same priority it had before) so that it can be assigned a new node.

As these changes do impact the way users interact with the `/scratch/local` file system, we will announce when they will be made. We anticipate starting this in January 2020. In addition, we will not make the change on all of the clusters at one time, but will instead make it on one or two at first, to give users time to adapt to the changes. Users will have to adjust any batch scripts or workflows that currently use the local scratch space so that they no longer try to write to or create directories under `/scratch/local` but instead write to `/scratch/local/$USER/$SLURM_JOB_ID`. If you need assistance in making this change, please reach out to CHPC staff by opening a ticket ([helpdesk@chpc.utah.edu](mailto:helpdesk@chpc.utah.edu)).

## Ember Replacement

News and Updates · Martin Čuma and Anita Orendt

For sustainability reasons—in terms of both datacenter space and power consumption—we are in the process of planning for the replacement of ember. Taking cost-to-performance into consideration, we are looking at servers that will each have a single AMD Rome 64-core processor (the 7702P) from the recently announced second-generation AMD EPYC 7002 Series.

The current ember cluster has a total of 143 nodes with a total of 2096 cores. Of these, 73 are general nodes (876 cores) and the remainder are owned by research groups. These nodes range from 6 to over 9 years old and the majority of these nodes contain two Intel Westmere processors with 6 cores per processor.

In terms of rack space, ember occupies six racks. We can essentially replace the core count with 32 nodes, each with 64 cores, which will occupy one-half of a rack when configured as high density “4 in 2U” units (4 nodes in a 2U unit). As we are close to capacity in the space we have available in the CHPC DDC machine room, this recovered space will allow for additional expansion.

In terms of power consumption, each of the two Westmere processors in an ember node has a power consumption of 95 watts, or 190 W per node for the processors, whereas the single AMD Rome 64-core processor has a power consumption of 200 W. Estimations are that this replacement will reduce the overall power consumption by over 300,000 kWh per year, which translates to a power cost savings of about \$25,000 per year. The power saving alone over the warranty life of these will nearly pay for the cost of these new nodes!

Note that while we are talking a replacement based on the core count, the newer cores have much higher computational capability. While CHPC Staff Scientist Martin Čuma is still in the process of completing a benchmark study on the new AMD Rome processor family, we do have a few early results to share in this newsletter. Once the benchmarking is complete, a final report will be posted on the CHPC website at [https://www.chpc.utah.edu/documentation/white\\_papers/index.php](https://www.chpc.utah.edu/documentation/white_papers/index.php). CHPC gratefully acknowledges Dell for providing access to AMD processor-based servers to allow us to complete this study.

The first comparison uses the HPCC benchmark, a synthetic benchmark suite geared at assessing different aspects of HPC performance. The HPCC consists of seven main benchmarks that stress various computer subsystems, such as raw performance, memory access, and communication. The results are given in the table above. Of specific note are the two highlighted columns: the HPL\_Tflops and the

Metric	Value	
Year	2019	2010
CPU generation	Rome 64	Westmere
Core count	64	2x6
Frequency_GHz	2	2.8
<b>HPL_Tflops</b>	<b>1.63</b>	<b>0.12</b>
StarDGEMM_Gflops	27.80	10.46
<b>SingleDGEMM_Gflops</b>	<b>49.20</b>	<b>10.71</b>
PTRANS_GB/s	11.56	3.05
MPIRandomAccess_GUPs	0.23	0.04
StarRandomAccess_GUPs	0.00	0.02
SingleRandomAccess_GUPs	0.12	0.04
StarSTREAM_Triad	1.62	2.48
SingleSTREAM_Triad	20.27	10.25
StarFFT_Gflops	0.95	1.22
SingleFFT_Gflops	1.59	1.95
MPIFFT_Gflops	24.97	4.64

single DGEMM\_Gflops. The first is the High Performance Linpack, which measures the floating point rate of execution for solving a linear system of equations; the result is given in TFLOPs (1 TFLOP is defined as  $10^{12}$  floating point operations per second) and is a measure of the whole-node performance. The second is a single-core run that measures the floating point rate of execution of double precision real matrix-matrix multiplication, and provides a measure of a single-core performance.

A second way to provide benchmark data is to run the real applications. At this point, we have the results for one application, the LAMMPS molecular dynamics program, which is widely used by researchers utilizing CHPC resources. Please note that LAMMPS is just one of the applications that will be used; other applications will not necessarily give the same results as LAMMPS.

Three LAMMPS benchmark cases are used:

- LJ = atomic fluid, Lennard-Jones potential with 2.5 sigma cutoff (55 neighbors per atom), NVE integration
- Chain = bead-spring polymer melt of 100-mer chains, FENE bonds and LJ pairwise interactions with a  $2^{1/6}$  sigma cutoff (5 neighbors per atom), NVE integration
- EAM = metallic solid, Cu EAM potential with 4.95 Angstrom cutoff (45 neighbors per atom), NVE integration

For this application, we are comparing the results from three systems: the existing ember nodes, the latest Intel-based notchpeak nodes, and the proposed AMD Rome processor-based nodes. In this case, the numbers are the run time in seconds, so lower is better.

There are two comparisons we can make from these results. The first is the performance gain between ember

and the proposed AMD nodes. The single-core performance is less than one-half as slow as the AMD CPUs, which is

Case	Scale	Runtime (s)		
		New AMD Nodes Single AMD Rome 7702P 64 cores per node	Latest Notchpeak Nodes Dual Intel Cascade Lake Gold 6230 40 cores per node	Current Ember Nodes Dual Intel Westmere X5660 12 cores per node
Chain	1 core	78.71	71.21	126.51
	1 node	1.47	2.32	12.95
EAM	1 core	354.38	294.20	640.14
	1 node	7.25	11.44	60.63
LJ	1 core	134.81	115.33	240.15
	1 node	2.82	4.39	24.64

understandable since LAMMPS does not take advantage of the vectorization as much as the dense linear algebra problems in the HPL or DGEMM. The speedup per node (12 vs. 64 cores) is eight to nine times.

The second comparison is between the AMD node and the latest Intel Cascade Lake notchpeak nodes. While the per-core performance favors the Intel processor, the per-node comparison favors the AMD due to the higher core count. Factoring in price, the AMD is a better value; our current vendor price for a 40-core Cascade Lake node is approximately \$5,100 while the 64-core AMD Rome server under consideration is about \$5,300.

## Plan for Replacement

We anticipate placing the order for nodes in early November and expect that the new nodes will be in production in early 2020. Once the new nodes are in service, the current ember cluster will be retired. CHPC will be contacting all groups that own ember nodes to discuss the retirement process.

At this same time, the general nodes of the kingspeak cluster will be taken off allocation. The net result of this, along with the expansion of lonepeak, discussed in the “Upcoming Changes to Lonepeak” article in this newsletter, is that there will be a growth in the number of core hours on general resources available, both those run unallocated as well as those run via our allocation system.

Current General Core Count		Planned General Core Count	
Allocated		Allocated	
Cluster	Cores	Cluster	Cores
notchpeak	1116	notchpeak	3164
kingspeak	832		
<b>Total</b>	<b>1948</b>	<b>Total</b>	<b>3164</b>
Unallocated		Unallocated	
Cluster	Cores	Cluster	Cores
ember	876	kingspeak	832
lonepeak	1100	lonepeak	2560
<b>Total</b>	<b>1976</b>	<b>Total</b>	<b>3392</b>

## Changes to Oracle Java

In July 2018, Oracle announced a change in their cost model for their Java products (Java SE) and support. While these products and the support have historically been free, the company moved to a subscription-based cost model effective January 2019 (date of last free public update and patch set for Java). This impacts the JRE (run-time environment) as well as the JDK (developer kit).

Note that this impacts access to Oracle Java version 8 or newer. Earlier versions of Oracle Java have already passed their end-of-life and therefore security patches are no longer being provided, making continued use a security risk (and a violation of university policy).

After evaluation options, the university purchased a one-time, 12-month Oracle Java subscription license that covers Oracle Java product use by main campus, Health Sciences, and University of Utah Health organizations, in order to give university organizations time to migrate to alternative no-cost Java products for in-house and vendor-provided software.

There are a number of free alternatives, including Oracle OpenJDK, AdoptOpenJDK, Amazon Corretto, Azul Zulu, and OpenJDK provided in Linux distributions.

All software requiring access to a Java installation at the University of Utah, regardless of operating system, will need to be individually assessed. This includes software being developed at the university, as well as commercial and open source software. This should be done by no later than May 2020 for security reasons, as the university will no longer have access to download patches for Oracle Java version 8 or newer. CHPC staff will be doing this for all software that we install and maintain, but users will need to do this for any software installations that are self-installed or self-maintained. If you need assistance, please send a request to [helpdesk@chpc.utah.edu](mailto:helpdesk@chpc.utah.edu).

For the University Information Technology (UIT) announcements, see the documents at [https://it.utah.edu/\\_downloads/public-announcements/2019-03-01%20java%20cost.pdf](https://it.utah.edu/_downloads/public-announcements/2019-03-01%20java%20cost.pdf) and [https://it.utah.edu/\\_downloads/public-announcements/2019-06-25-java-license.pdf](https://it.utah.edu/_downloads/public-announcements/2019-06-25-java-license.pdf).

A UIT Knowledge Base article explains alternatives and factors to consider: [https://uofu.service-now.com/it?id=uu\\_kb\\_article&sys\\_id=b06f3c2fdb8fff80a750d8f3ce9619a1](https://uofu.service-now.com/it?id=uu_kb_article&sys_id=b06f3c2fdb8fff80a750d8f3ce9619a1).

A UIT Brown Bag Lunch recording and slides are also available (contact CHPC if you are unable to access this): <https://uofu.app.box.com/s/egahf7ibxugibduv3s0yvmukoq1x5bdv>.

The UIT contact for questions regarding this change is Brad Millett ([brad.millett@hsc.utah.edu](mailto:brad.millett@hsc.utah.edu)).



The University of Utah  
University Information Technology  
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