The High Performance Computing Newsletter For SMU

A Word from the Director

We are living in a time where computing is at the center of both progress and fear throughout society. Will artificial intelligence make us safer, more prosperous, and free from toil or will it be a tool of disruption, doubt, and chaos? That these questions can even arise is an amazement to me given the fundamental simplicity of the underlying models and algorithms, which are typically built on functions we all studied in middle school or high school, combined with relatively straightforward and somewhat random data-fitting. John von Neumann, a great mathematician of the previous century who was extremely influential in the early development of computers, is quoted as saying "With four parameters I can fit an elephant, and with five I can make him wiggle his trunk". The famous/infamous ChatGPT model has hundreds of billions! We have seen the incredible results a model of this complexity can achieve, but, unlike the small models we call laws of nature, it makes its behavior difficult to predict or to understand.

Researchers here have been enjoying access to a tool specifically designed for developing and training large-scale AI models – our NVIDIA DGX SuperPOD. In this newsletter, Kevin Brenner of the Department of Electrical and Computer Engineering describes his group's work on the quantum mechanics of sound and vibration, with simulations of the molecular dynamics enabled by the SuperPOD. Besides the SuperPOD, we are excited to announce the availability of ManeFrame III, our new CPU cluster. I also want to congratulate two of the Center's faculty fellows who received major awards in scientific software development at this year in Amsterdam at the Society of Industrial and Applied Mathematics biennial conference on Computational Science and Engineering. Devin Matthews of the Department of Chemistry, with a colleague from UT Austin, was awarded the James H. Wilkinson Prize for Numerical Software. Dan Reynolds of the Department of Mathematics is part of a team which was awarded the SIAM/ACM Prize in Computational Science and Engineering.

Lastly, I want to thank the fantastic staff who keep the machines running, consult with researchers at all levels, and all in all make the Director's job an easy one: Amit Kumar and Richard England, our HPC Systems gurus, Rob Kalescky and John Lagrone who provide user support, and Lauren Gilmore, the program coordinator for the CRC as well as the Data Science Institute. Best wishes for a productive summer!

Tom Hagstrom

Center for Research Computing (CRC) Director

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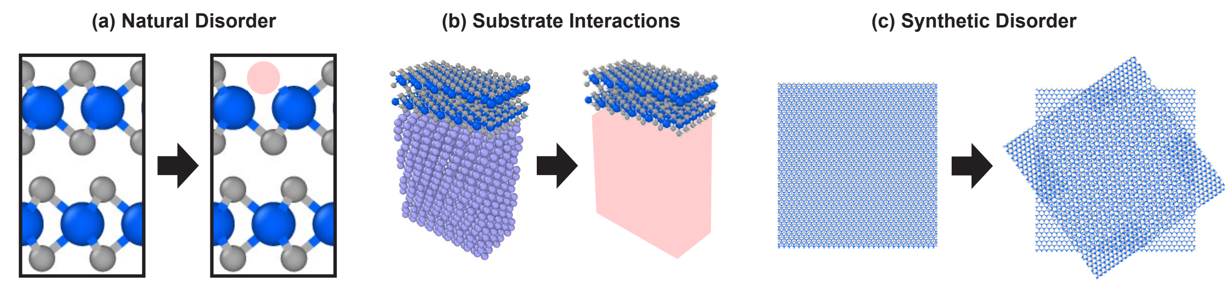
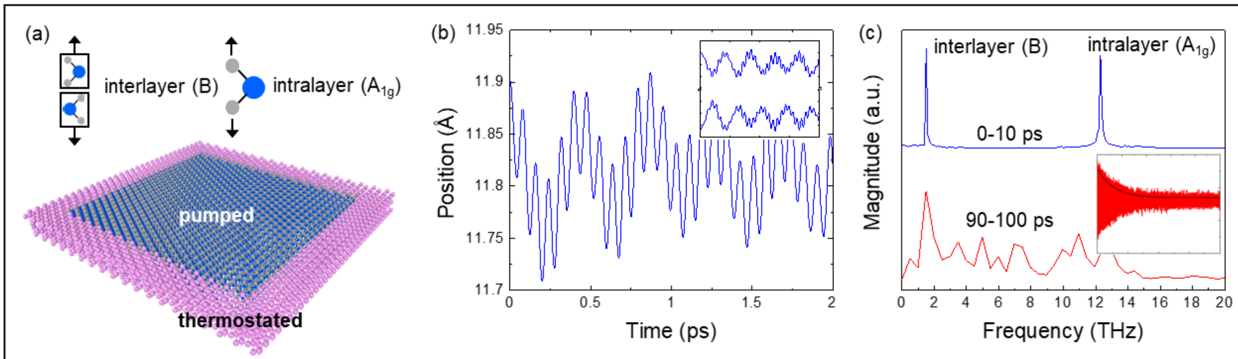
Tapping into the Quantum Nature of Phonons with Molecular Dynamics Simulations

The dynamics of vibrations in crystals are driven by many fundamental aspects of the underlying chemistry. Treating these vibrations as harmonic oscillators, the mass of the atoms and the stiffness of the chemical interaction between the atoms determines the period of oscillation. In crystals, these collective vibrations become waves called phonons. An equilibrated crystal with phononic energy will have a distribution of thermal phonons (TPs), filling lower-energy modes first and lacking coherence. However, when imparting this energy on timescales much shorter than the phonon period (femtosecond range), it is possible to create a nonequilibrium distribution of specific phonon modes in phase. This can be done with femtosecond laser pumps. These coherent phonons (CPs) are akin to Raman scattering, and through various processes, will ultimately equilibrate into TPs. Understanding how chemical disorder drives this equilibration is a fundamental challenge for tapping into the quantum nature of phonons.



Various types of structural and chemical disorder than can be imparted into our molecular dynamics simulations.

The geometry that is often used to experimentally probe CPs is a thin film. Here, the film's surfaces function as phononic mirrors that reflect the CPs, thus forming a mechanical resonator. A pump-probe setup can then measure the coherence of the resonator through time-resolved changes in reflectivity or transmission. These resonators are also significant as their frequency and quality factor – a measure of their coherence – determine the temperature at which their quantum ground state may be observed. Layered crystals may significantly advance our control over CPs as they offer unprecedented tailoring of the thickness, interfaces, and disorder that may be applied to a resonator. For example, layered transition metal dichalcogenides (TMDs), where CPs of the Raman-active breathing mode(s) can be pumped and probe. However, the large spatial complexity and diverse (bonded and nonbonded) chemical interactions of TMDs have made it difficult to establish fundamental relationships between disorder and the equilibration of CPs. While first-principles modeling has predicted the intrinsic (anharmonic) lifetimes of phonons in TMDs, we have only scratched the surface of how disorder drives CPs, and their precursory role in valuable structural transitions or metastable states not possible in equilibrium conditions. Our work is developing approach-to-equilibrium molecular dynamics (AEMD) frameworks, run on the DGX Superpods, for understanding how various forms of structure and chemical disorder drive the equilibration process.



Our AEMD framework for investigating CPs in TMDs. (a) A ~ 10 nm × ~ 10 nm bilayer of MoS_2. Center atoms are pumped via expansion of the breathing modes, while the edges are thermostated to ambient temperature. (b) Tracking atomic displacements to reveal the superposition of the interlayer (B) and intralayer (A_{1g}) breathing modes. Inset shows the average motions of the two layers matching the B mode. (c) Spectral analysis of the raw atomic displacements during the first (0-10) and last (90-100) picoseconds of the simulation. The frequency of the B and A_{1g} modes dominate the coherent regime. Inset shows the time-dependent temperature as the resonator decays from a harmonic oscillator to thermal equilibrium.

Summer Bit Blast

Last summer three CRC Faculty Fellows: Tom Coan from Physics, Harsha Gangammanavar from OREM, and Eojin Han from OREM designed and delivered a two-week-long short course on coding and applications to a group of eight area high school students. The students wrote programs in Python and R with applications ranging from word games to chaos to data science. This summer the same group of faculty will partner with the Simmons School's College Access Upward Bound program to get more local students exposed to the wonders of computing and the mathematics behind it.

Photo by: Guillermo Vasquez

Highlights from the CRC Annual Report on HPC Utilization

- There were 464 active users
- 11 million jobs submitted
- More than 100 grants and grant proposals were supported
- Chemistry led the way with the most jobs submitted followed by Physics, History, Biology and Economics
- Chemistry also led the way in the most processing hours used followed by Earth Sciences, Mechanical Engineering, Statistical Science, Physics and Economics

Congratulations to Our 1st Graduating Class of CSE Fellows!

The Center is delighted to congratulate our first graduates of the fellowship program in Computational Science and Engineering, who will be awarded their doctoral degrees this May. They are:

- Eric Guzman, Department of Physics, "Deep Learning Applications For Secondary Cosmic Microwave Background Anisotropies" (advisor Joel Meyers)

- Megan Simons, Department of Chemistry, "New Methods for Core-Hole Spectroscopy Based on Coupled Cluster Theory" (advisor Devin Matthews)

In addition, three other fellows plan to schedule their defenses for the summer: Niloofar Fadavi from the Department of Operations Research and Engineering Management, Yanling Lin from the Department of Electrical and Computer Engineering, and Mateus Quintano from the Department of Chemistry. Next year, four fellows will be part of the group: Bin Huang from the Department of Electrical and Computer Engineering, Shuo Qi from the Department of Economics, Sian Xiao from the Department of Chemistry, and Elyssa Sliheet from the Department of Mathematics. It has been a pleasure meeting with the fellows and sharing their research interests.

Supercomputing 22 in Dallas Computing Day 2023

Supercomputing 22, the premier International Conference for High Performance Computing, Networking, Storage, and Analysis was held at the convention center in Dallas this past November. SMU's booth featured videos highlighting our world-class computational infrastructure and a slideshow describing some of the HPC-enabled research projects across campus. Many of the graduate fellows were able to attend as well as OIT's Research Computing and HPC Systems groups. As often is the case, the student-build Jetson cluster was one of the booth's main attractions.

ManeFrame III and NIVIDIA SuperPOD

In this past year SMU has installed two new state-of-the-art facilities which provide a many-fold increase in computing power compared with ManeFrame II, which will be retired over the summer. In combination these provide faculty, students and partners access to hardware unmatched at any University our size.

By now I hope many of you have had a chance to try out our NVIDIA DGX SuperPod, which became operational last summer. The SuperPOD architecture is specifically designed for artificial intelligence applications, but it can also be exploited to accelerate traditional numerical algorithms. The SuperPOD consists of twenty nodes each containing eight A100 GPUs connected by a fast network. It is only the second SuperPOD to be installed at an American university and it presents a unique opportunity for SMU researchers. If you haven't used it yet, but are intrigued by the possibility of applying AI tools in your research, keep an eye out for the excellent workshops provided by OIT's Research Technology Services team, or ask them directly for a consultation session.

To complement the GPU-based SuperPOD, a CPU-based cluster, ManeFrame III, is now ready to roll. With more than 25000 cores, ManeFrame III has more than twice the raw computing power of ManeFrame II, with a network which is also twice as fast. ManeFrame II users will have their data migrated by staff over the coming weeks. We expect this process to be complete by the end of June.

	M2	M3	SuperPOD
Nodes	354	200	20
CPU Cores	11,276	25,600	2,560
GPU Cores	275,968		1,392,640
Memory	120TB	112TB	52.5TB
Nodal Interconnect	100GB/S	200GB/S	200GB/S
Storage	3.6PB	8.0PB	768TB

Research Computing Day 2023

The Center held its second Research Computing Day on April 21 at the Hughes-Trigg Student Center. More than 70 people registered to attend from both inside and outside the University. The program included two keynote addresses: Jeff Hittinger, Director of the Center for Applied Scientific Computing at Lawrence Livermore National Lab gave a talk entitled ``Is Fusion Our Future? (Yes, but maybe not the way you think.)" and Mark Austin, Vice President for Data Science at AT&T gave a talk entitled ``Democratization of Data and AI and Applied Use Cases at AT&T". In addition there were excellent presentations by SMU faculty: Devin Matthews from Chemistry, Corey Clark from the Guildhall and Computer Science, Allison Deiana from Physics, Jianhui Wang from Electrical Engineering, Harsha Gangammanavar from OREM, Andrea Barreiro from Mathematics, Ali Beskok from Mechanical Engineering, and Mitch Thornton from Electrical Engineering and the Darwin Deason Institute for Cyber Security, along with poster presentations from SMU graduate students.

Special thanks to Lauren Gilmore and Tim Angell for organizing and publicizing the event and to NVIDIA and Mark III Systems for their sponsorship.

Photo by: Marek Freindorf