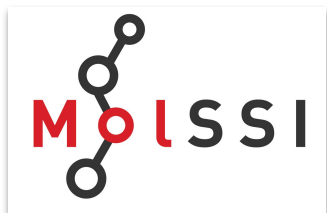


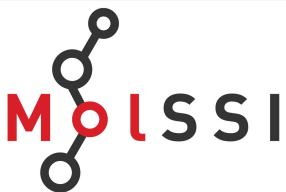
# Sustainability definition

Theresa Windus  
Iowa State University  
Ames Laboratory  
[twindus@iastate.edu](mailto:twindus@iastate.edu)



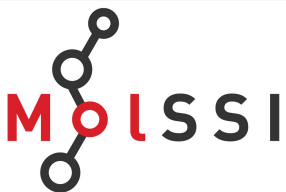
# What is sustainable software?

- Dan Katz blog 09/13/2016: “Here I offer a quick definition of sustainability in the context of software: **the capacity of the software to endure**. In other words, **sustainability means that the software will continue to be available in the future, on new platforms, meeting new needs.**”
- Patricia Lago at [WSSSPE4](#) with tweaks from Neil Chue Hong  
Sustainable software is software which is:
  - Easy to evolve and maintain
  - Fulfils its intent over time
  - Survives uncertainty
  - Supports relevant concerns (Political, Economic, Social, Technical, Legal, Environmental)



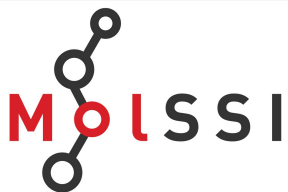
# What is sustainable software?

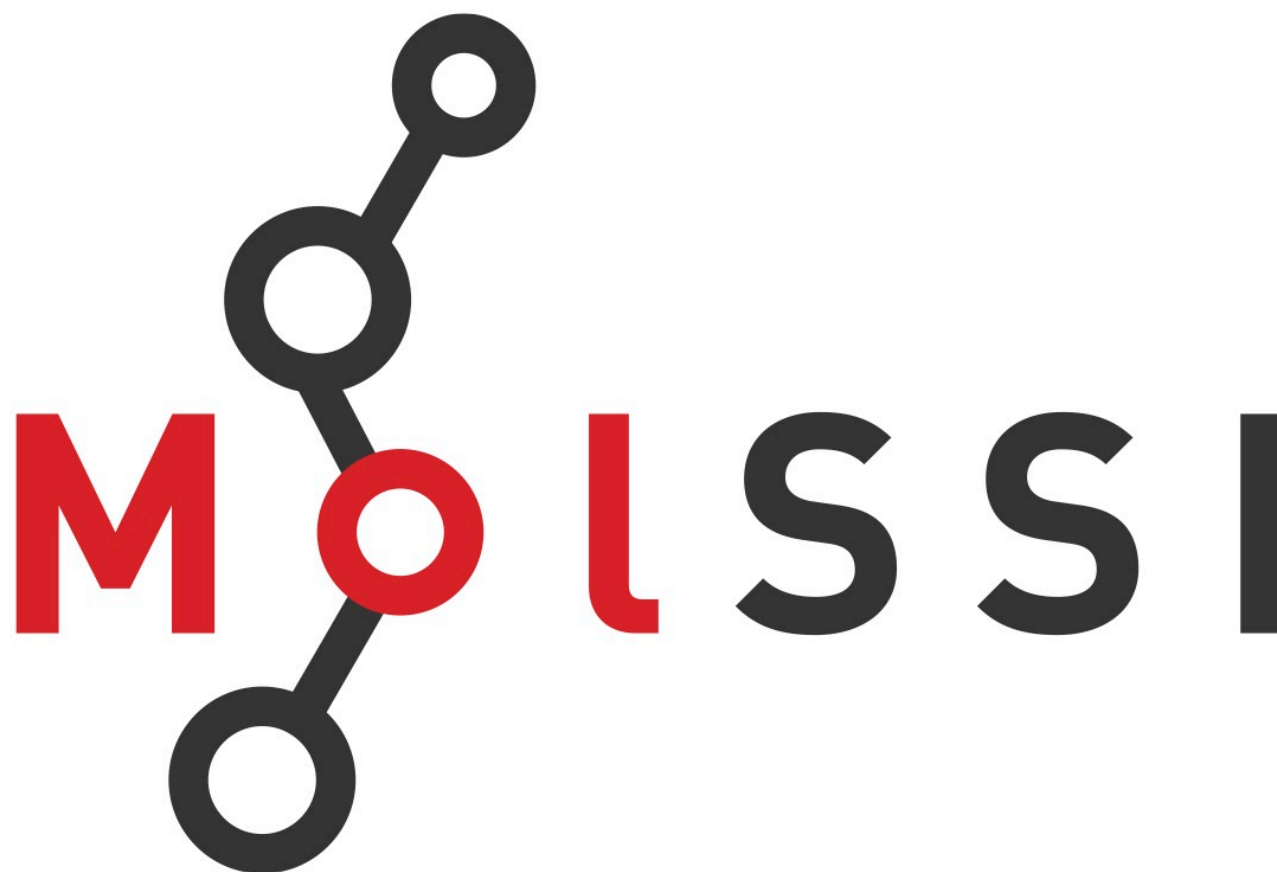
- <http://catalogue.pearsoned.co.uk/samplechapter/0321286081.pdf>  
“Sustainable software development is a mindset (principles) and an accompanying set of practices that enable a team to achieve and maintain an optimal development pace indefinitely. ”
- Robert Heine in <https://www.energypedia-consult.com/en/blog/robert-heine/what-sustainable-software> “The concept of sustainability is based on three pillars: the ecological, the economical and the social. This means that for a software to be sustainable, we must take all of its effects – direct and indirect – on the environment, the economy and the society into account. In addition, the entire life cycle of a software has to be considered: from planning and conception to programming, distribution, installation, usage and disposal.”



# What is sustainable software?

- Joost Visser in <https://www.infoq.com/news/2018/04/sustainable-software-agile/> *“So for software, “sustainable” actually means “evolvable”.”*
- Tom Dufour in <https://www.infoq.com/news/2018/04/sustainable-software-agile/> *“To me, it is software that can be understood quickly and can be edited easily.”*

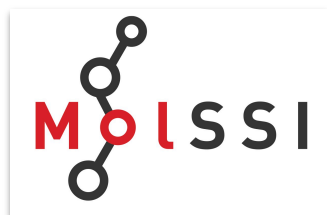




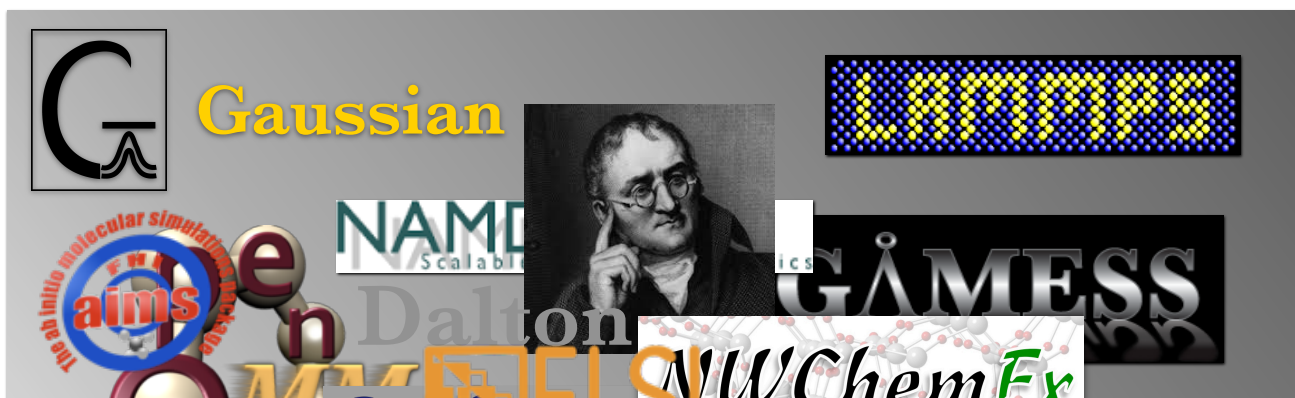
## **The Molecular Sciences Software Institute**

... a nexus for science, education, and cooperation for the global computational molecular sciences community.

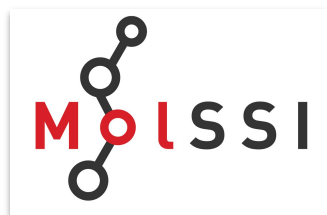
# Codes Are Developed and Used Globally



# Codes Are Developed and Used Globally

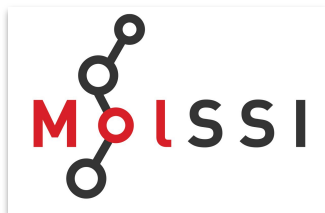


These codes represent **decades** of development by thousands of programmers, and are used by **hundreds of thousands** of scientists worldwide.



# Code Complexity and Historical Legacy

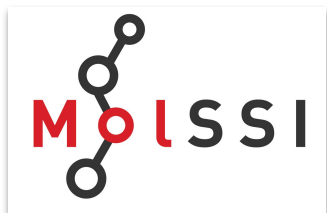
- CMS programs contain **millions of lines of hand-written code** and require **hundreds of programmers** to develop and maintain.
- Incredible **language diversity**: F77, F90, F95, HPF, C, C++, C++11, C++14, C++17, Python, perl, Javascript, etc.
- Incredible **algorithmic diversity**: structured and unstructured grids, dense and sparse linear algebra, graph traversal, fast Fourier transforms, MapReduce, and more.
- The packages have evolved in an ad hoc manner **over decades** because of the intricacy of the scientific problems they are designed to solve.





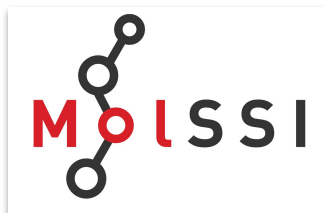
# Rapidly Evolving Computing Hardware

- **Multi- and many-core architectures** are the norm, but many CMS codes are developed with limited view to parallel task management.
- Reduced-power solutions will also require improved **error recovery and checkpointing** at the software level – capabilities absent in nearly all CMS codes.
- Anticipated architectural innovations will yield **even greater hardware complexity** – more advanced accelerators, specialized computing cores, reconfigurable logic...
- Many CMS codes (especially for quantum chemistry) are limited to shared-memory paradigms and cannot yet take advantage of GPUs or **large-scale distributed-memory systems**.



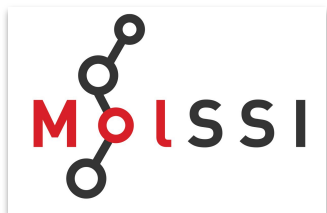
# Some examples of unsustainability

- **No plan for design** – no thought to modularity, separation of concerns, reusability, extensibility, or ease of use. Just get the job done.
- **Picking the wrong horse in the language/library race** – perl and Fortran examples; which on-node parallel library to use (OpenMP, OpenAcc, CUDA, Kokkos)
- **Programming too close to the hardware** – assembly as the extreme
- **Programming too abstractly** – can't get performance on any hardware
- **Inefficient usage of resources** – hardware and human
- **Lack of well defined interfaces** – multiple implementations that don't get used; FFT example



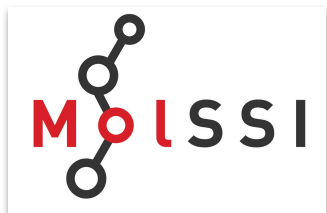
# Some examples of unsustainability

- **Lack of code development oversight** – may have rules, but if not enforced...
- **Depending on other libraries** – especially if they are not sustainable; version control nightmare
- **No or very little documentation** – both user and developer
- **Inadequate testing** – Just get the job done; potential incorrect results for other users
- **Lack of user communication during development** – Might have a great idea, but if doesn't meet the end user need, then it hasn't served its purpose
- **Single point of failure** – Hit by a bus syndrome



# Not all software should be sustained

- **Society has evolved past the use of the software** – software no longer meets a specific need
- **Training** – software will not be good the first time and is likely highly redundant
- **Prototype** – often is used as the final solution, but that is not its original purpose
- **Software should die gracefully** – Zach Mathew  
<https://medium.com/building-freshbooks/great-software-isn-t-built-to-last-it-s-built-to-die-gracefully-594df9c3a470>



# Acknowledgments

- T. Daniel Crawford; the Board of Directors, and the wonderful MolSSI staff scientists;
- The NWChem and NWChemEx developers;
- The dozens of members of the CMS community who helped to develop the vision;
- NSF ACI-1547580;
- Exascale Computing Project

