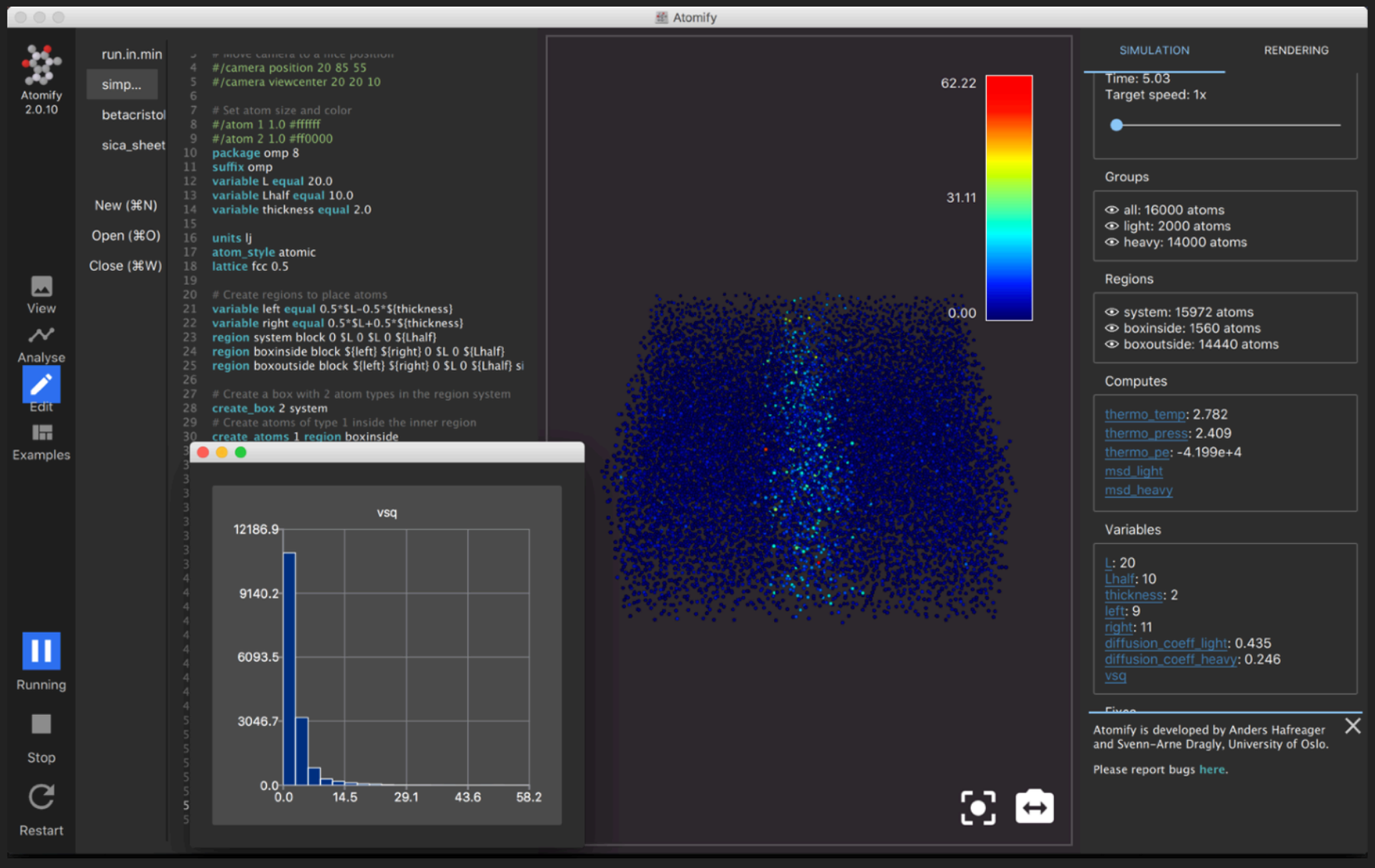

INCREASED PRODUCTIVITY WITH REAL TIME VISUALIZATION

ATOMIFY

Anders Hafreager and Svenn-Arne Dragly
University of Oslo, Norway

“I´M NOT GOING TO SHAVE UNTIL I HAVE LEARNED LAMMPS”

76% male LAMMPS beginners [1]

[1] bit.ly/lammps-survey

“I’M NOT GOIN
UNTIL I HAVE
LAMMPS”

76% male LAMMPS beginners [1]

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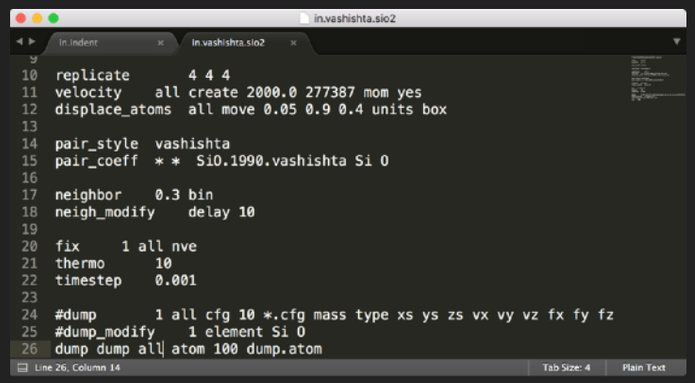
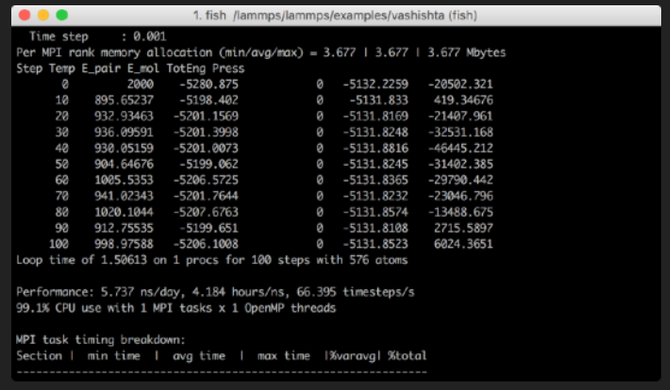
DOWNLOAD FROM BIT.LY/ATOMIFY

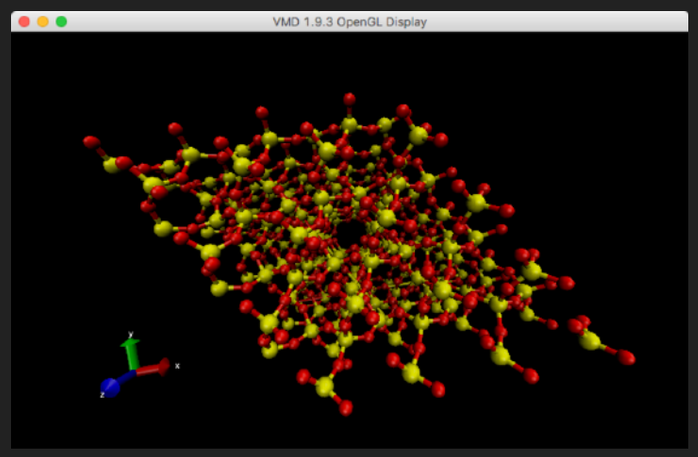
LAMMPS WORKFLOW INCLUDES MULTIPLE PROGRAMS



Editor to write scripts



Terminal to run LAMMPS



VMD/Ovito to visualize

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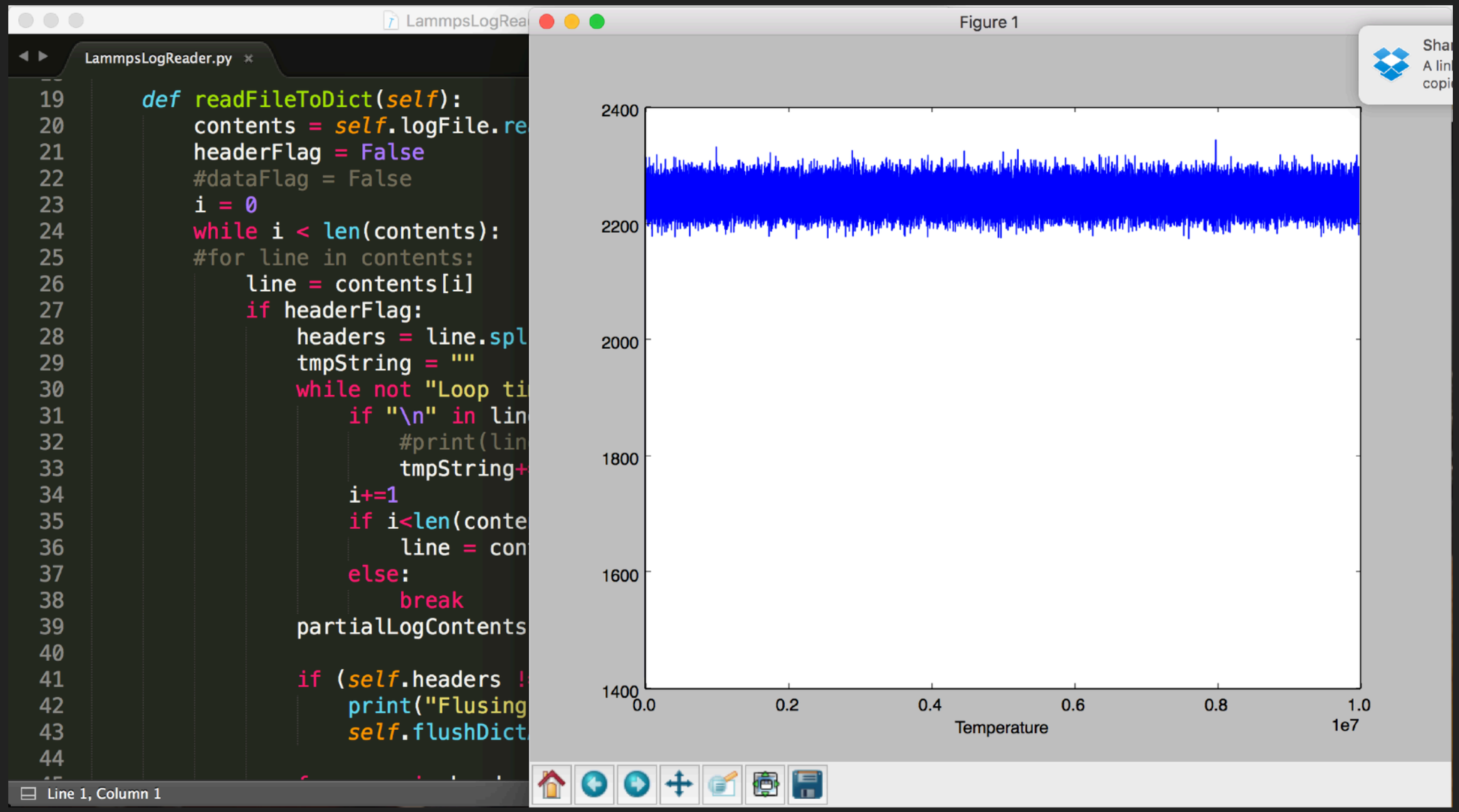
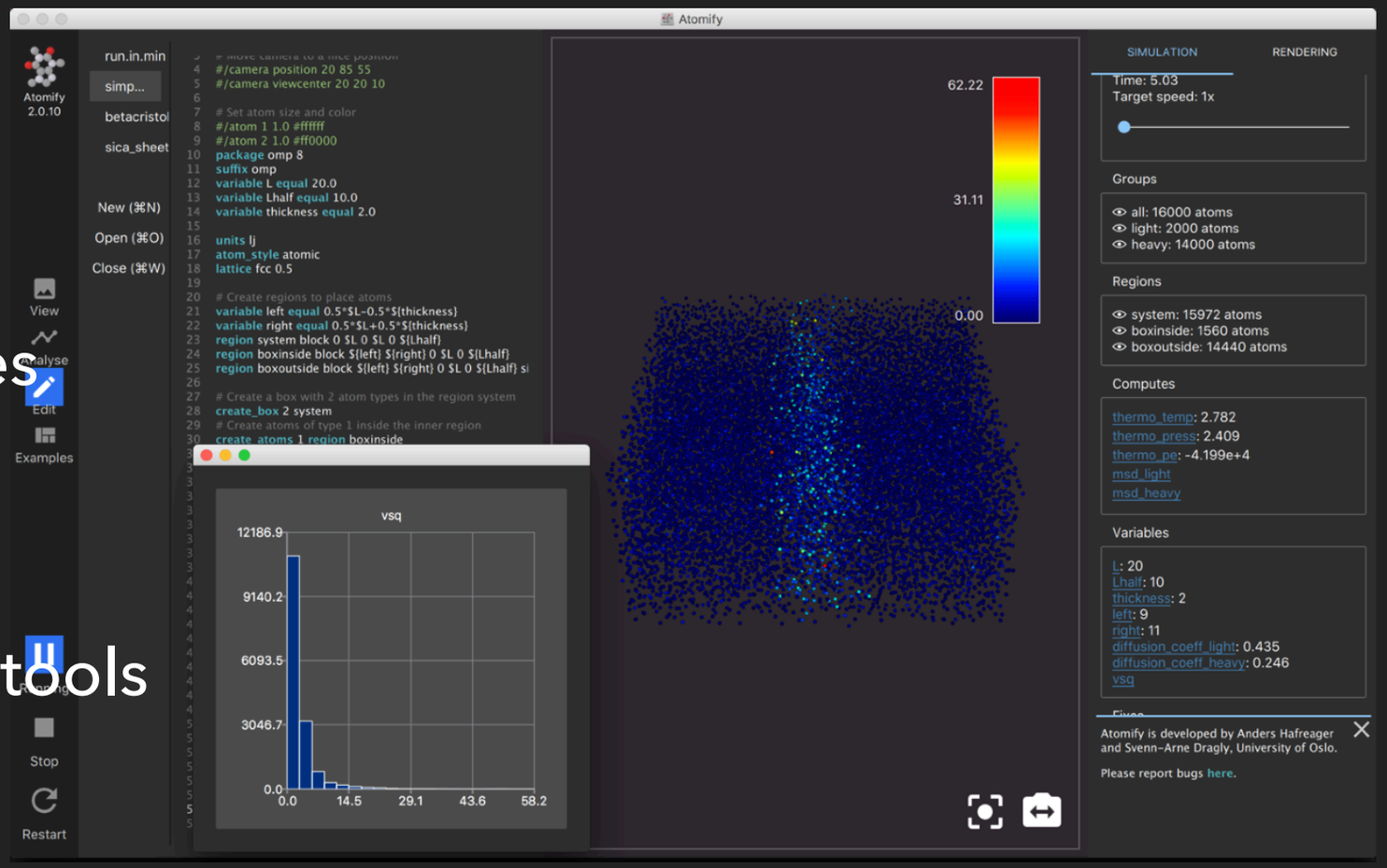
WHAT ABOUT PLOTTING?



DOWNLOAD FROM [BIT.LY/ATOMIFY](bit.ly/atomify)

ATOMIFY

- Uses LAMMPS as a library
- Real time visualization
- Supports accelerator packages
- Built with Qt (c++)
- Not trying to replace existing tools (VMD/Ovito)



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DEMO

DOWNLOAD FROM BIT.LY/ATOMIFY

WHAT CAN IT BE USED FOR?

- Especially good for learning purposes
- Script prototyping
- With powerful desktop GPU's production runs can be performed
- I've run 10000 atoms, 1 microsecond with vashishta manybody potential (1xNVidia GP100, double precision)

C++ COMPILES TO ALL PLATFORMS

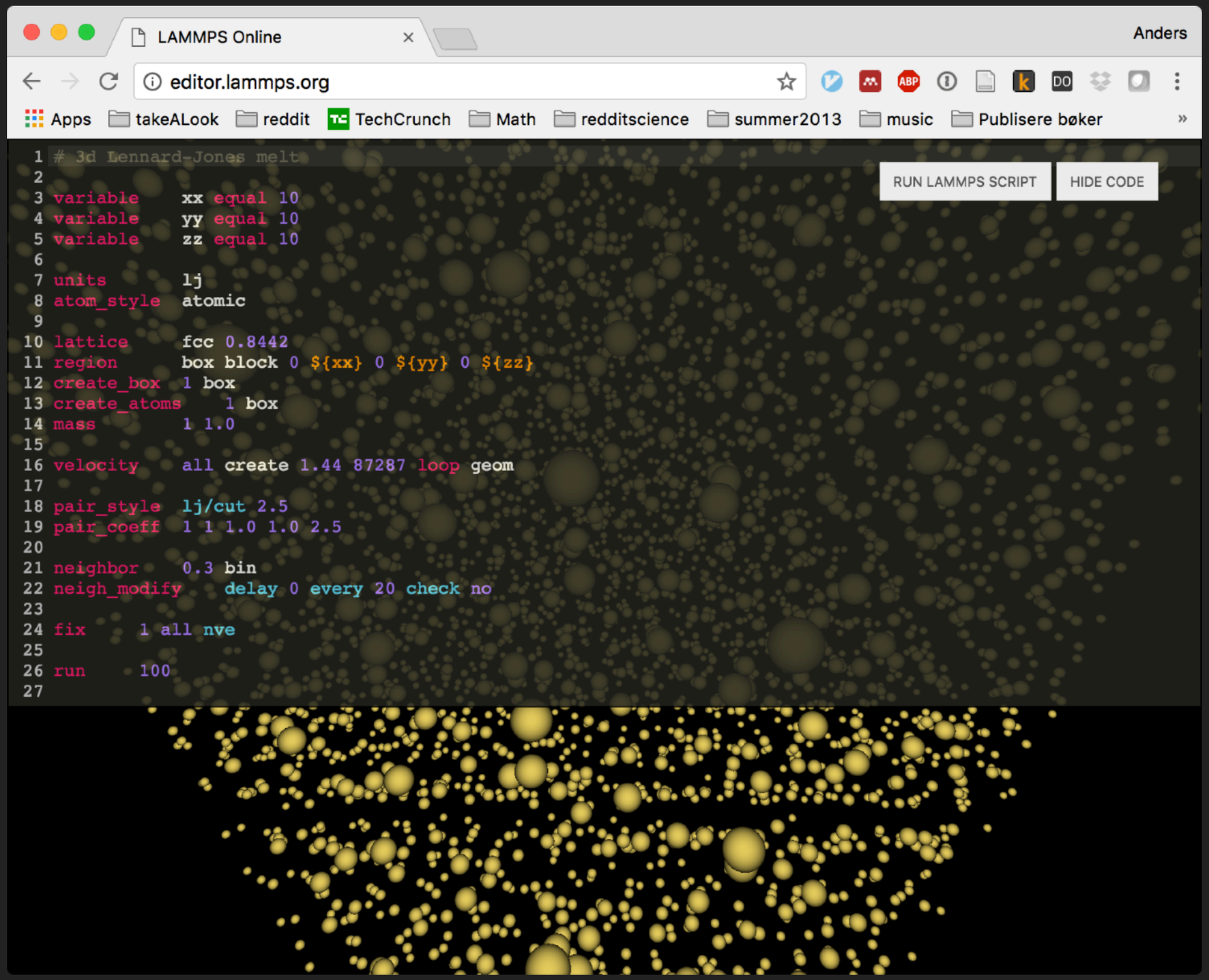
- Run LAMMPS on your phone/tablet
- Free in App Store for both iOS and Android
- We need more systems! Do you have scripts that could be cool?

AND BTW, HAS ANYONE HEARD ABOUT EMSCRIPTEN AND ASM.JS/WEBASSEMBLY?

C++ COMPILES TO JAVASCRIPT WITH EMSCRIPTEN…

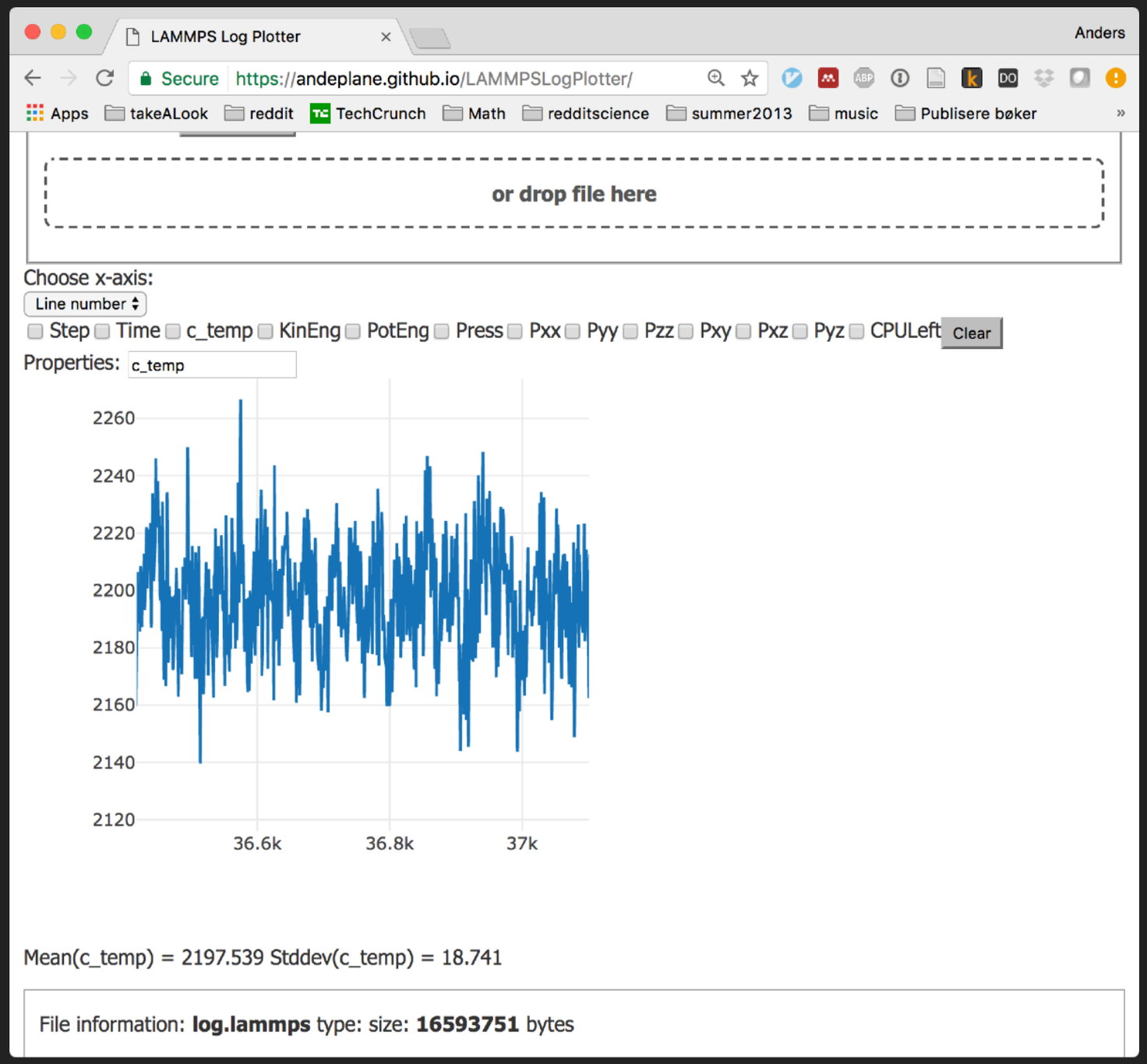
TRY IT AT [EDITOR.LAMMPS.ORG](editor.lammps.org)

C++ COMPILES TO JAVASCRIPT WITH EMSCRIPTEN...



TRY IT AT [BIT.LY/LOGPLOTTER](bit.ly/logplotter)

EASY PLOTTING OF LOG FILES

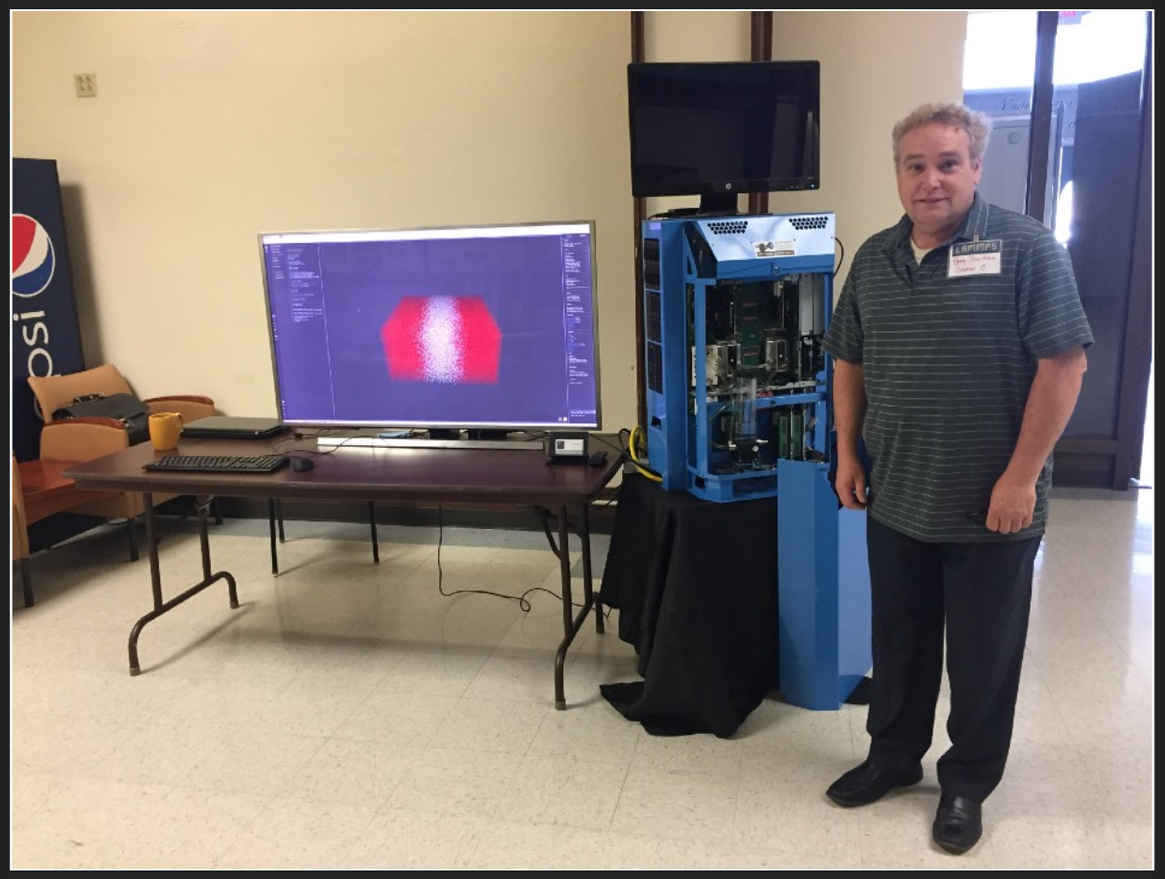


DOWNLOAD FROM BIT.LY/ATOMIFY

IF YOU WANT TO TRY

- Phone/tablet version of Atomify is free in iOS / Android app stores
- Download Atomify for macOS or Ubuntu: github.com/ovilab/atomify or bit.ly/atomify
- Web version: editor.lammps.org
- Log plotter: bit.ly/logplotter
- **Feedback is extremely appreciated!**

Thank you!
(sorry, I had to)



Check out the demo during lunch!
(thanks Greg)