LAMMPS on GPUs

A Tutorial

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Why run on GPUs?

- Technology paid for by gamers, but impact to scientific computing is now well-recognized
- Cheap, low-power (electrical) solution for data parallelism
  - 240+ cores on a GPU
  - High memory bandwidth

Porting LAMMPS to GPUs

- Still largely a research effort

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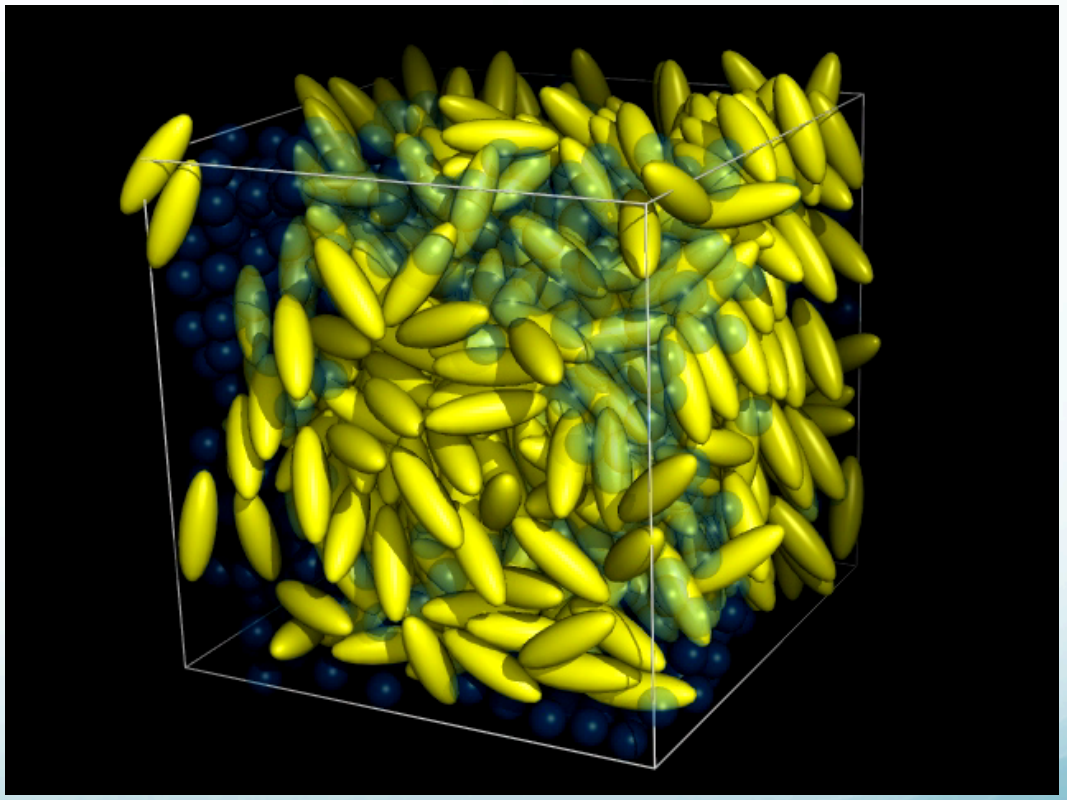
Currently Available in "Main" LAMMPS

- Lennard-Jones
  - Force/Neighbor
- Gay-Berne Potential
  - Force
- More capabilities soon...



How to Run LAMMPS on Your GPU

1. Do you have a GPU?

- For single precision
  - Currently need a CUDA-enabled GPU with compute capability >= 1.1
- For double precision
  - Currently need a CUDA-enabled GPU with compute capability >= 1.3

Windows: Device Manager
Apple: "Apple Menu"-> "About this Mac" -> "More Info" -> "Graphics/Displays"
Linux: `nvidia_settings` or `/sbin/lspci | grep nVidia`

List of CUDA-enabled GPUs here:
http://www.nvidia.com/object/cuda_gpus.html

Can use device query to get compute capability; more later...

2. Do you have CUDA?

- http://developer.nvidia.com/object/cuda_2_3_downloads.html
  - Need driver and toolkit only
  - Need to have the `nvcc` compiler in your path
  - *Pay attention to 32- or 64-bit*
    - No 64-bit on apple!

```
set path = ( $path /usr/local/cuda/bin )
setenv LD_LIBRARY_PATH /usr/local/cuda/lib/

or

set path = ( $path /usr/local/cuda/bin )
setenv LD_LIBRARY_PATH /usr/local/cuda/lib64/
```

3. Edit LAMMPS GPU Makefile

```
set LROOT = "/home/wmbrown/lammps-20Feb10"
cd $LROOT/lib/gpu
emacs Makefile.nvidia
```

3. Edit LAMMPS GPU Makefile (2)

```
BIN_DIR = .
OBJ_DIR = .
AR = ar
CUDA_CPP  = nvcc -I/usr/local/cuda/include -DUNIX -O3 -Xptxas -v --
use_fast_math
CUDA_ARCH = -arch=sm_13
CUDA_PREC = -D_SINGLE_SINGLE
CUDA_LINK = -L/usr/local/cuda/lib64 -lcudart $(CUDA_LIB)
```

For compute capability >= 1.3 can also use:

```
CUDA_PREC = -D_SINGLE_DOUBLE # Double precision accumulation
or
CUDA_PREC = -D_DOUBLE_DOUBLE # Double precision everything
```

For Apple, must compile 32-bit

```
CUDA_ARCH = -arch=sm_13 -m32
CUDA_LINK = -L/usr/local/cuda/lib -lcudart $(CUDA_LIB)
```

For compiler >= g++ 4.4 on Linux

```
CUDA_ARCH = -arch=sm_13 --compiler-bindir=/usr/bin/gcc-4.3
```

4. Make LAMMPS GPU lib

```
make -f Makefile.nvidia
./nvc_get_devices
```

```
Device 0: "GeForce GTX 295"
  Revision number:                               1.3
  Total amount of global memory:                 0.87 GB
  Number of multiprocessors:                     30
  Number of cores:                               240
  Total amount of constant memory:               65536 bytes
  Total amount of shared memory per block:       16384 bytes
  Total number of registers available per block: 16384
  Warp size:                                     32
  Maximum number of threads per block:           512
  Maximum sizes of each dimension of a block:    512 x 512 x 64
  Maximum sizes of each dimension of a grid:     65535 x 65535 x 1
  Maximum memory pitch:                          262144 bytes
  Texture alignment:                             256 bytes
  Clock rate:                                    1.24 GHz
  Concurrent copy and execution:                 Yes

Device 1: "Tesla C1060"
```

5. Edit LAMMPS Makefile as Necessary

```
cd $LROOT/src
emacs ./MAKE/Makefile.linux
```

If you are not 64-bit (or Apple)

```
gpu_SYSPATH =       -L/usr/local/cuda/lib
```

If you are using Apple, compile LAMMPS 32-bit to link with GPU library

```
CC =        g++ -m32
LINK =      g++ -m32
```

```
make clean
```

6. Add GPU Package to LAMMPS

```
cd $LROOT/src
make yes-asphere
make yes-gpu
make linux
```

7. Modify your input script

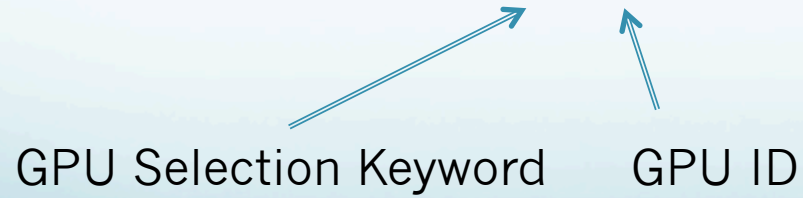
```
cd $LROOT/bench
emacs in.lj
```

Must add '`newton off`' to beginning of script and '`/gpu`' to a supported pair_style

```
newton off

...

pair_style lj/cut/gpu one/node 0 2.5
```



7. Modify your input script (2)

- GPU Selection Keyword
  - **one/node** - single compute "node", which may have multiple cores and/or GPUs. *GpuID* should be set to the ID of the (first) GPU you wish to use with LAMMPS
  - **one/gpu -** multiple compute "nodes" with one GPU per node. *GpuID* should be set to the ID of the GPU.
  - **multi/gpu -** multiple compute "nodes" on your system with multiple GPUs. *GpuID* should be set to the number of GPUs per node

8. Run your input script

- **Number of procs = number of gpus you want**

```
mpirun -np 3 lmp_linux < in.lj
```

```
-----------------------------------------------------------------------
- Using GPGPU acceleration for LJ-Cut:
-----------------------------------------------------------------------
GPU 1: Tesla C1060, 240 cores, 4 GB, 1.3 GHZ
GPU 2: Tesla C1060, 240 cores, 4 GB, 1.3 GHZ
GPU 3: GeForce GTX 295, 240 cores, 0.87 GB, 1.2 GHZ
-----------------------------------------------------------------------
```

```
-----------------------------------------------------------------------
      GPU Time Stamps:
-----------------------------------------------------------------------
Atom copy:      0.07111 s.
Neighbor copy: 0.0004615 s.
LJ calc:        0.1702 s.
Answer copy:    0 s.
-----------------------------------------------------------------------
```

9. Speed-ups

- Depends on
  - Your CPU
  - Your GPU
  - Number of Particles
  - Cutoff
- More talks showing the GPU acceleration in LAMMPS to come...

Questions