Autogenerating gpu-accelerated LAMMPS pair styles

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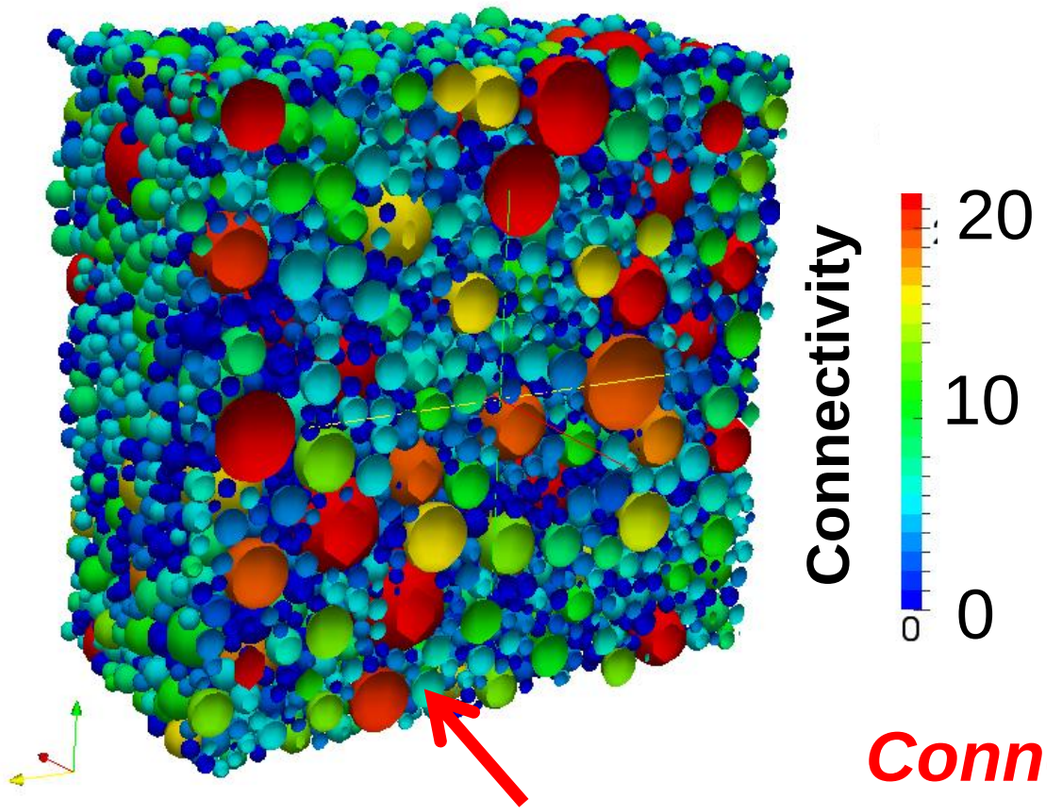
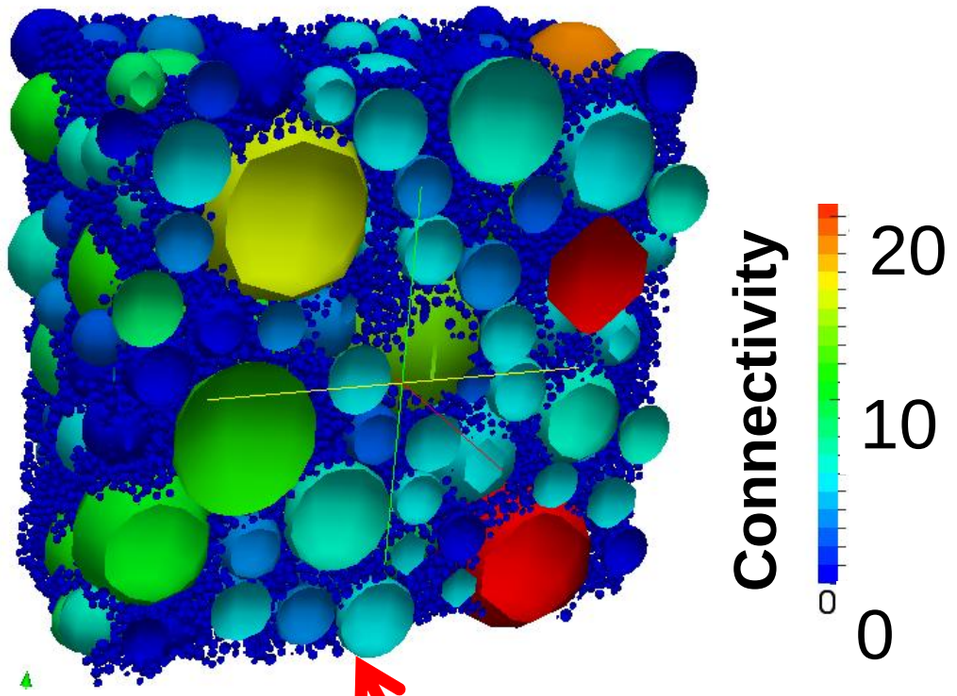
Doing experiments...



Stable dam filter

Connectivity = number of contacts a particle has with other contacts



Unstable dam filter

Using DEM to develop a rational basis for dam filter design

vs. writing experiments

```
__global__ void bpp_compute_kernel(
  int nparticles,
#ifdef AOS_LAYOUT
  struct particle *particle_aos,
#else
  struct particle particle_soa,
#endif
  int *numneigh, double *force, double *torque
#ifdef NEWTON_THIRD
  , double3 *fdelta, double3 *tdeltaj
#endif  ) {
  __shared__ double ftmp[NSLOT*3];
  __shared__ double ttmp[NSLOT*3];
  int jj = threadIdx.x; int idx = blockIdx.x;
  if (idx < nparticles && jj < numneigh[idx]) { ... }
```

Implementation details

- CPU or GPU?
- Choice of decomposition
- Data-layout and orchestration
- Algorithm tradeoffs
- Effective use of resources

Hardware choices

- Intel SCCC, MIC
- AMD Fusion
- NVIDIA Fermi, Kepler, Maxwell

Opportunity for Software Optimization Group

- Targeting granular community of LAMMPS
- Make it easy to write pair styles that execute with good performance on a variety of hardware platforms

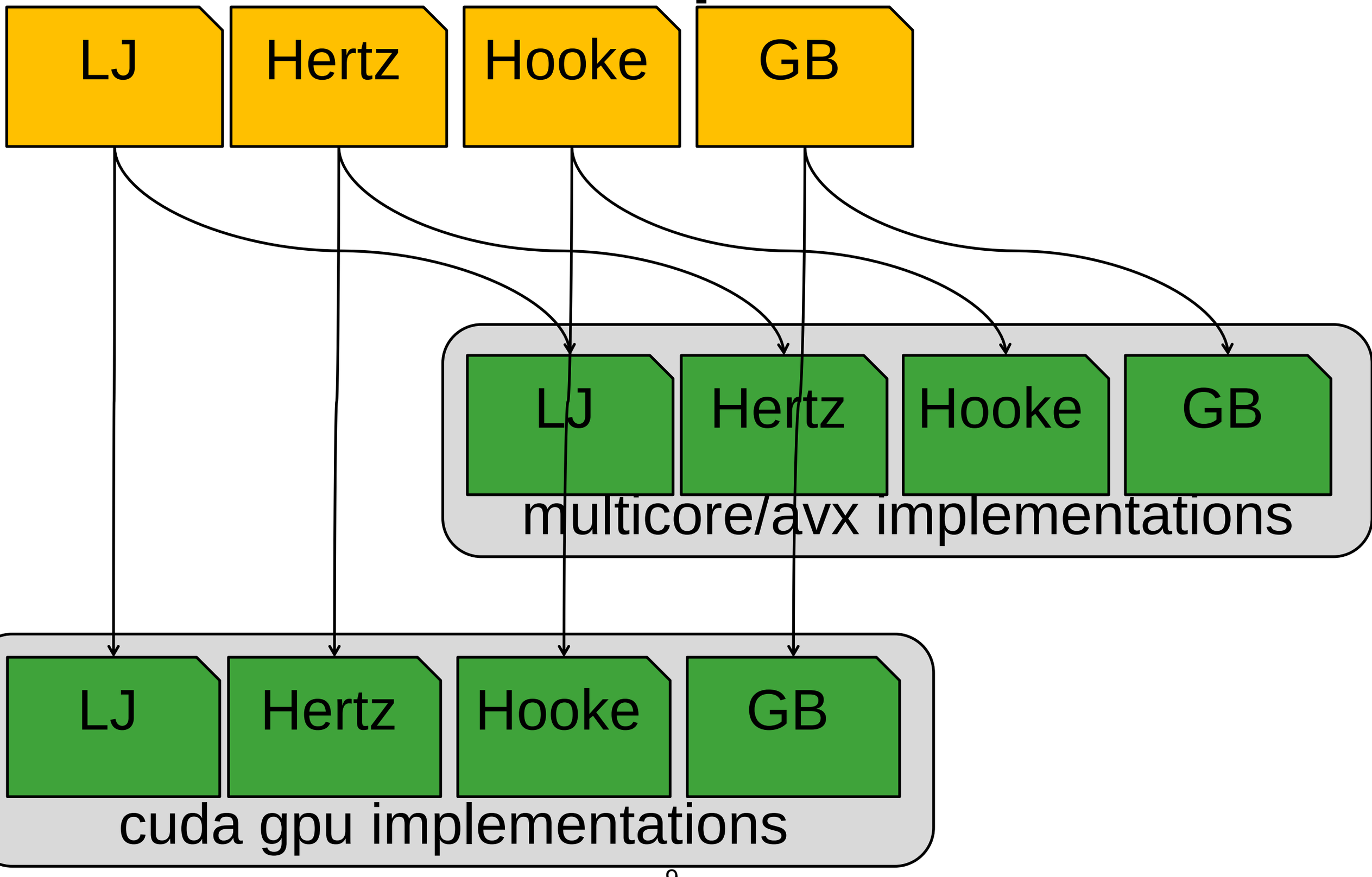
Key idea: abstraction

- Separate specification and implementation
  - pairwise interaction (mechanical model)
  - data/access pattern
  - implementation details (eg, how to decompose the problem onto parallel hardware)

Related work

- Molecular Dynamics: OpenMM, NAMD
- Unstructured Grid: OP2, Liszt
- Other: SPIRAL, FFTW, ATLAS

The NxM problem



Abstraction

LJ | Hertz | Hooke | GB

Simple, abstract specifications

pairgen

LJ | Hertz | Hooke | GB

multicore/avx implementations

LJ | Hertz | Hooke | GB

cuda gpu implementations

Step 1. Create parameter file

```
name: hertz
parameters:
  - name: x
    type: double
    arity: 3
    set: P
    access: RO
  - name: v
  - name: omega
  - name: radius
    arity: 1
  - name: mass
    arity: 1
name: type
    arity: 1
    type: int
  - name: force
    access: SUM
  - name: torque
    access: SUM
  - name: shear
    set: N
    access: RW
constants:
  - name: dt
  - name: nktv2p
  - name: yeff
  - name: geff
  - name: betaeff
```

Step 1. Create parameter file

We invoke pairgen at
the command line:

```
$ pairgen.py hertz.yml
```

Step 2. Add detail to generated code

```
__device__ void hertz_pair_kernel(
 double xi[3], double xj[3],
  double vi[3], double vj[3],
  double omegai[3], double omegaj[3],
  double radiusi, double radiusj,
  double massi, double massj,
  int typei, int typej,
  double forcei_delta[3],
  double torquei_delta[3],
  double shear[3],
  int *touch) {
 //fill me in
}
```

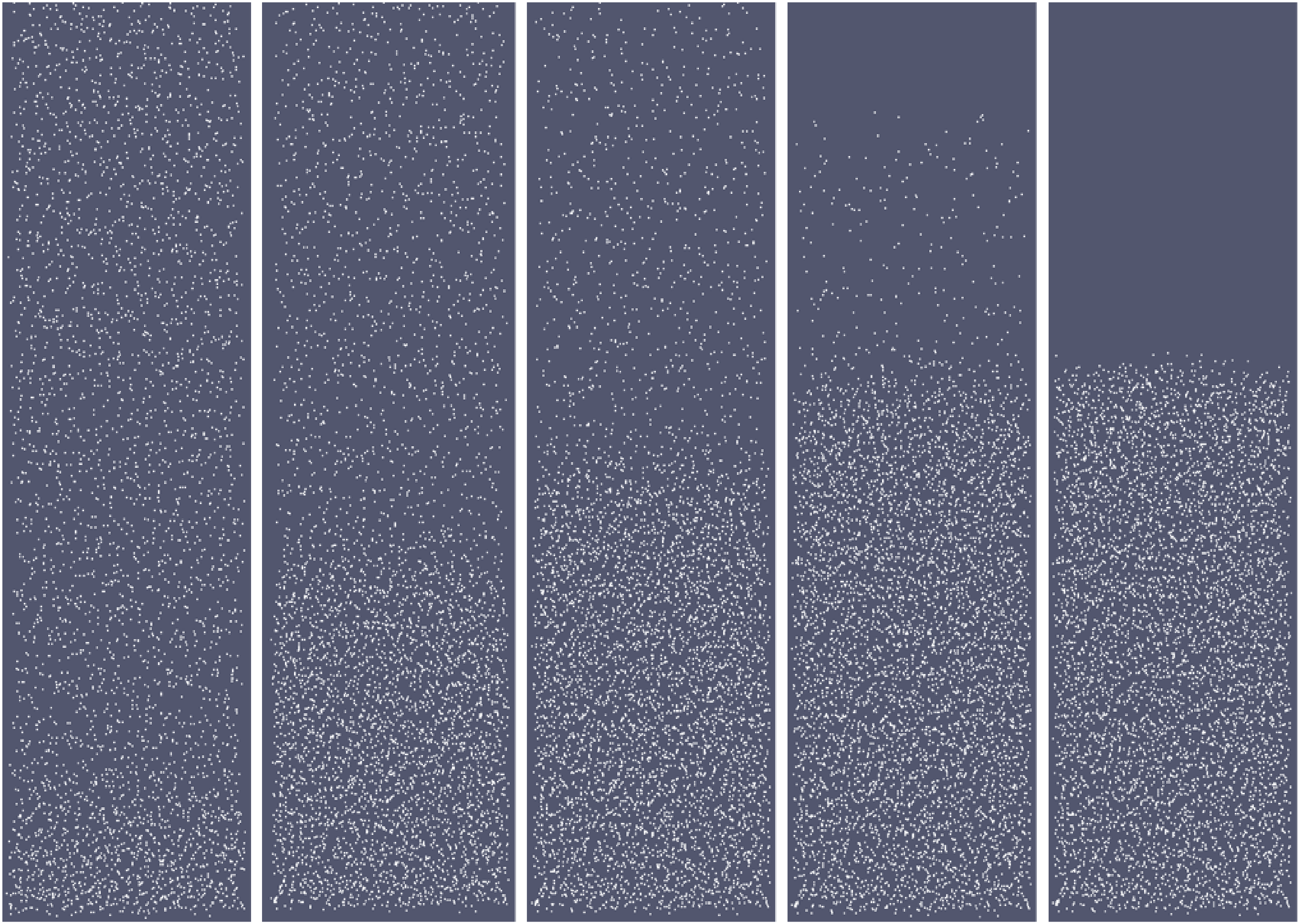

hertz_kernel.cu

Step 3. Autogenerated pairgen output (implementation)

```
__global__ void bpp_compute_kernel(
  int nparticles,
#ifdef AOS_LAYOUT
  struct particle *particle_aos,
#else
  struct particle particle_soa,
#endif
  int *numneigh, double *force, double *torque
#ifdef NEWTON_THIRD
  , double3 *fdelta, double3 *tdeltaj
#endif  ) {
  __shared__ double ftmp[NSLOT*3];
  __shared__ double ttmp[NSLOT*3];
  int jj = threadIdx.x; int idx = blockIdx.x;
  if (idx < nparticles && jj < numneigh[idx]) { ... }
```

Experimental evaluation

- Simulation data taken from raining of particles into a box under gravity
- Constant number of particles, 45.6K
- Number of neighbors increases as simulation proceeds
- Vary number of neighbors for problem size

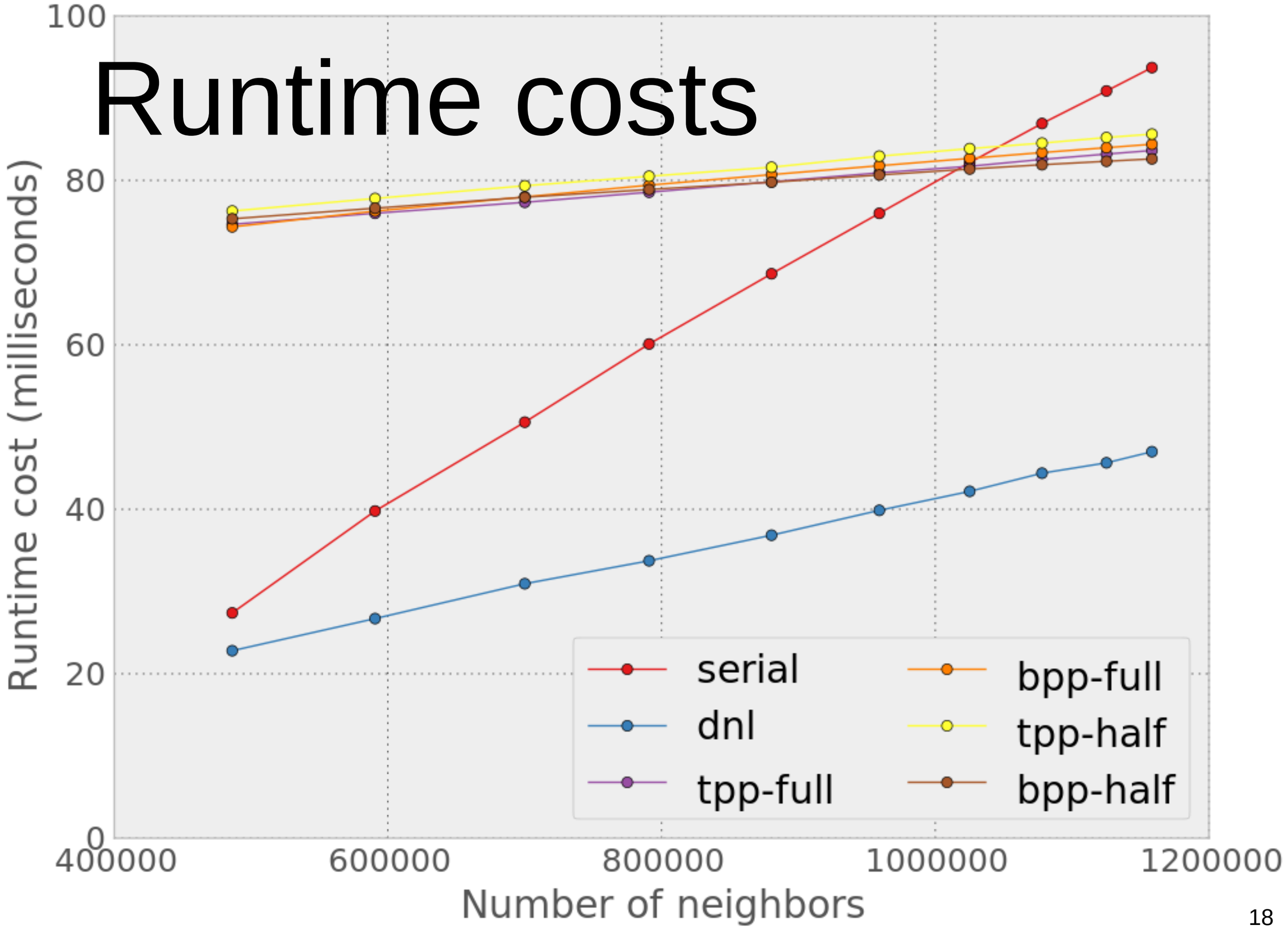


Implementations

Using pairgen

	Neighbor list datastructure	Decomposition	Neighbor list
serial	None	n/a	Half
dnl	Dense-neighbor	Thread per neighbor	Half
tpp-full	Sparse-neighbor	Thread per particle	Full
bpp-full	Sparse-neighbor	Block per particle	Full
tpp-half	Sparse-neighbor	Thread per particle	Half
bpp-half	Sparse-neighbor	Block per particle	Half

Runtime costs



Conclusions

- Make it easy to write pair styles that execute with good performance on a variety of hardware platforms
- Pairgen addresses abstraction and performance (but not yet performance portability)

Future work

- Modifying pairgen to achieve a dense neighbour implementation *(ongoing)*
- Generating implementations for different hardware
- Extending this domain-specific approach to other parts of the LAMMPS simulation loop (in particular, fixes).
- Dynamically switching between implementation choices as simulation characteristics change

Nathan Chong

- http://www.doc.ic.ac.uk/nyc04/
- nyc04@doc.ic.ac.uk
- Please email for information on test driving pairgen!

Experiment details

Toolset

	Version	Flags
g++	4.4.3	-O2
nvcc	3.2	-arch sm_13

Hardware

- Intel P4 3.6GHz
  - 2GB memory
- NVidia GeForce GTX 480 (Fermi)
  - 1.5GB global memory
  - 15 multiprocessors/120 cores