Developers/Hackers Breakout Session

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2nd LAMMPS Workshop
August 2011 - Albuquerque, NM

Agenda

- Steve: quick tutorial on how to modify LAMMPS (15 min)
- Axel: setup (VMD), monitoring (IMD), analysis (VMD) (15 min)
- Everyone: discussion of possible new features (75 min)
  - recap from yesterday
  - mail list postings
  - your suggestions
  - planning
  - someone to take notes?

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- Thinking about a "developers" manual
  - describe code structure, underlying algorithms in LAMMPS
  - unfortunately a lot of work, low priority
  - good idea?

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  - force fields = pair style, bond, angle, dihedral, improper
  - long range = kspace style
  - fix = fix style = BC, constraint, time integration, ...
  - diagnostics = compute style (global, per-atom, local)
  - geometric region = region style
  - output = dump style
  - minimizer = min style
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- Enabled by C++
  - virtual parent class defines interface
  - new child class implements the methods

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- Find an existing style that does something similar
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  - especially important if you want to do something complex
    - does functionality you want already exist?
    - is it a good idea to do this in LAMMPS?
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- Understand how that style works and is structured
  - examine parent class header file (e.g. pair.h)
  - look at other *.cpp and *.h files for that style
  - doc/Section_modify.html
  - if you get stuck, post to mail list

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  - fame and fortune, name on author page and in source code
  - acquire "users" of your feature
    - find and fix bugs
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- Are there things we could do to make development easier?

Axel's presentation

Use of VMD and IMD with LAMMPS

Requests for new features in these or other pre/post processing tools?

New features planned from yesterday's talk

- Core/shell potential (Mike Chandross, Sandia)
- COMP potential (generation 3) (Ray Shan, U Florida)
- MGPT potential (Jaime Marian, LLNL)
- BOP potential (Don Ward, Sandia)
- GAP potentials (Aidan Thompson, Sandia)
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- LIGGGHTS integration (Christoph Kloss, JKU)
- AtC enhancements (Reese Jones, Jeremy Templeton, Jon Zimmerman, Sandia)
- GPU enhancements (Mike Brown, ORNL) (Christian Trott, U Tech Ilmenau)
- Long-range solvers (Paul Crozier, Stephen Bond, Sandia)
- SPH (Georg Ganzenmüller, Franhofer-Institute, EMI)

User ideas from mail list solicitation

- Radiation damage potential of Giovanni (2011) for FeCr (Agraj Abhishek)
- Pair_style table/density for CG potentials (Tim Sirk)
- V-rescale thermostat of Bussi (Vasili Artyuknov)

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  - better restart file format
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  - Complexity of building code?
  - Something you wish was easier to do?
  - Something you can't do?
  - Something another MD code can do?
  - Performance issues?
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- What are your suggestions & ideas?