

Breakout session: Developers brainstorm

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LAMMPS resources for code development

- Website
 - Workshops page
 - slides (PDF) for Developers breakout at Aug15 and Aug13 workshops
 - Git and GitHub tutorial (PDF) at this years workshop
 - Developer Guide (PDF) = some details on code structure
- Manual
 - Section 10 = Modifying & Extending LAMMPS
 - Section 10.15 = guidelines for submitting code to LAMMPS
- Python
 - Section 11 = Python interface to LAMMPS
 - variable python = define a **variable** that invokes Python code
 - fix python = define a **fix** that invokes Python code
 - pair_style python = define a **pair style** with Python code
 - **python** = define Python code in-line or in a file

LAMMPS resources (continued)

- **GitHub**

- link on LAMMPS website
- branches: master, stable, unstable
- <https://github.com/lammps/lammps/issues>
bugs, new features, discussion, etc
- <https://github.com/lammps/lammps/pulls>

- **Mail list**

- link on LAMMPS website
- hosted on SourceForge, archived by SF, also LAMMPS website
- Google search, e.g. fix npt lammps-users
- post brief message about what you want to do
 - feature may already exist
 - may be someone already working on it
 - get advice about how to go about it
 - get advice on how to make it LAMMPS compatible
- good idea if want to eventually contribute it to LAMMPS

Working on new CMake option for building LAMMPS

- Christoph Junghans (LANL)
- Richard Berger (Temple U)

Coming attractions: work in progress

- **Hyperdynamics**, global and local
 - with Art Voter, Danny Perez (LANL)
 - accelerated time algorithm, bond-boost variant
 - applicable to solids: distinct basins, rare events
 - speed-up can be dramatic, depending on energy barrier heights & temperature
 - parallel implementations, currently testing
- **Fix react** command
 - Jake Gissinger (U Colorado)
 - define reaction **templates** = before/after topologies
 - define reaction **criteria**: probability or Boltzmann or rates
 - allow for dynamic **relaxation** after bond change
 - superset of fix bond/create and fix bond/break
- **Granular media** enhancements
 - with Dan Bolintineanu (Sandia), Trung Nguyen (Northwestern)
 - aspherical particles (rounded-edge polyhedra)
 - **triangulated surfaces** as boundaries or sharp-edged particles
 - some overlap with LIGGGHTS

Open discussion

- What are your **questions**?
- What are your **complaints**?
- What are your **suggestions** for new features?
- What is a **new feature** you're working on?