



NOVEL MATERIALS DISCOVERY

European Center of Excellence



NOMAD CoE receives funding from the European Union's Horizon program under the grant agreement N° 951786.



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TaskBlaster

TaskBlaster is a light-weight system to execute computational workflows

- Workflow: Python class which declares methods that specify tasks
- Task: Target function and associated inputs, such as future output of other task
- Storage of tasks in directory tree supported by lightweight (sqlite) database for lookups
- Access via directory tree is intuitive, easy to inspect
- Tasks are invalidated if inputs (from workflow) are modified; validation of a task based on hashing its inputs
- Extensibility via Python plugin





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TaskBlaster

More on TaskBlaster:

- Command-line interface provides operations on tasks:
Run, submit, “unrun”/remove, and list information in different ways
- Workflow managers (slurm/torque/...) supported using myqueue
- Tasks generally executed by running workers; workers acquire and execute multiple available tasks, can generate more tasks
- Currently used for certain projects related to Atomic Simulation Recipes (ASR)
- Plugin (ASR-level) support for ASE objects, internal (Python) MPI, ...





LUMI “Hero run”

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Large scaling test to LUMI supercomputer

- LUMI is a GPU-based supercomputer
- Benchmark of TaskBlaster workflow with relaxations and ground-state calculations by GPAW
- Many difficulties: LUMI downtime and scheduling combined with version-dependent software bugs sometimes deep in software stack
- Successful use of full LUMI during final hour of six-hour window





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ASE interfaces for workflows

Work on “ase-engines” at DTU March 2023 hackathon

- Generalization of electronic structure code interfaces in Atomic Simulation Environment (ASE)
- Current calculator interfaces are designed for dynamics: Energy, forces, stresses
- New standardized interfaces necessary for other simulation types
- New mechanisms required for multi-step calculations
- Without these interfaces, workflows become very code dependent and brittle
- Design in draft stage, needs refactoring and more iterations
- Functioning integration tests with multiple codes on gitlab



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Conclusions

- TaskBlaster works but is still changing significantly
- Would be wise to continue work on ase-engines project



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