ScalaLife

Scalable Software Services for Life Science

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KTH

WP3 – Description and Organization

Setting up infrastructure
for porting and maintenance of
GROMACS, DALTON and DISCRETE

Deliverables

Deliverable Number	Deliverable Title	Estimated indicative person-months	Delivery date
D3.1	Project software releases with documentation	28	12
D3.2	Project software releases with documentation	28	24
D3.3	Project software releases with documentation	28	21
D3.4	Report on integration of results from WP6 and WP7	14	36

D3.1) Public release of new version of the three software packages together with installation and usage documentation.

D3.4) This report provides a detailed analysis of the improvements achieved by integrating the results from WP6 and WP7.

Achievements

- Milestone 13: Development versions available to WP4
- Software / traces provided to WP6 for analysis
- Continued work on parallelization

GROMACS: classical molecular dynamics

	Milestone name	Delivery date	
MS13	Development version available to WP4	6	Feeds into D3.1
MS14	Software running on all project resources for validation by WP4	12	Feeds into D3.1
MS15	First split-level parallelization integrated	18	Feeds into D3.2 and D3.4
MS19	Dispatcher-queue based parallel versions of selected analysis tool available	24	Feeds into D3.3 and D3.4

GROMACS work

Based on results of tasks 6.1, 6.2, 7.2, and 7.3:

- New methods for separating direct and reciprocal space force calculation
- 2D domain decomposition for the 3D FFT
- Adapting communication patterns to hardware
- Subset of cores handles inter-node comm.
- Implement and maintain combination of MPI and thread pallelization for NUMA
- Multiple time stepping to reduce global comm.
- Parallelize analysis tools by dispatching trajectory frames

DALTON: QM and QM/MM computational platform

	Milestone name	Delivery date	
MS13	Development version available to WP4	6	Feeds into D3.1
MS14	Software running on all project resources for validation by WP4	12	Feeds into D3.1
MS16	Linear scaling DFT methodology for multicore CPUs available	18	Feeds into D3.2 and D3.4
MS20	Parallelization of linear scaling matrix/matrix and matrix/vector computational routines	30	Feeds into D3.3 and D3.4

Dalton work

Based on the results of task 6.5:

- Extension of linear scaling DFT for multi-core CPU nodes, involving parallelization of linear algebra and compact storage
- Design and implementation of QM/MM methods where MM is done one the GPU and QM on a multi-core CPU
- Development of object oriented tools for arithmetic evaluation of exchange-correlation functional derivatives

DISCRETE: coarse-grained, discrete MD

	Milestone name	Delivery date	
MS13	Development version available to WP4	6	Feeds into D3.1
MS14	Software running on all project resources for validation by WP4	12	Feeds into D3.1
MS18	High parallelization scaling version	24	Feeds into D3.3 and D3.4

DISCRETE work

Based on the results of task 6.1, 7.1 and 7.2:

- Implement and maintain performance improvements
- Integrate new interface and exchange standards
- Parallelization of collision events and porting to GPGPUs

Actual work

Question:

How much of the code development will be done in WP3 vs. WP6 and WP7?

The “release” work:

- Making new code work for all (supported) input parameters and/or systems
- Making new code work on all platforms
- Documentation in the code and user manual

Question:

What parts of the performance optimization (analysis, tuning etc.) belong to WP3, WP4 and WP6?

Managing releases

Possible issues with releases within ScalaLife

- What state of testing / reliability / polish?
- Documentation
- Download link accessible to everyone?
- Licensing issues (Dalton)
- If password protected, how does the user get a password?

Deadlines

- Deadline for software releases
- Deadline for reporting

Connection with WP6

- Have area's of potential improvement of parallelization been identified for Gromacs, Dalton and/or Discrete?

- What are the current plans & schedule for working on this in WP6?

Connection with WP2

- How to make new features know to the community?
- Ideally: developers talk at events, but flying over to talk 30 minutes?
- Suggestion: developers prepare presentations for WP2

Developer meeting

- A developer meeting is planned for 17:30 – 19:00