



Scalable Software Services for Life Science

WP6 – Scalable techniques Progress and Future Plans

Judit Gimenez - BSC



- Analysis and performance profiling of current life science codes
 - GROMACS, Dalton, and DISCRETE software packages
- Multi-level parallelization:
 - Multicore
 - GPU
 - Cluster
- Ensemble computing techniques
 - to break the “impossible” performance barrier on machines where there will be significantly more cores than particles in the system simulated

Planned tasks and efforts

T 6.1.	Analkysis				D6.1		D6.2
T 6.2	Parallelization				D6.1		D6.2
T 6.3	Ensemble						D6.2
T 6.4	Accelerators						D6.2
T 6.5	Mgmt						

	T 6.1	T 6.2.	T 6.3	T 6.4	T 6.5.		
	Analysis	Parallelization	Ensemble	Accelerators	Mgmt		Total
KTH	6	8	12	9			35
IRB							0
BSC	8	4	5		3		20
BADW	3	4	4				11
UOXF	4	14	10				28
SYN				8			8
Total	21	30	31	17	3		102

- **T6.1 Analysis and structure for efficient parallelization**
 - Keep analysing the 3 applications
 - Despite many sort of delays
 - Some WP6 partners cannot dedicate effort yet
 - Delays getting traces
 - DALTON now Xavi Aguilar obtains the traces
 - DISCRETE was on the oven
 - GROMACS analysis stopped until MPI+OpenMP ready (mid Jan), now getting traces trough ORNL
 - Enough material for many hours presentation

- T6.2 Multi-level/multi-scale parallelization
- T6.3 Ensemble computing techniques for scalability
- T6.4 Porting algorithms to accelerator architectures
 - Request to coordinate initial tasks on February 14th
 - Applications have been parallelised / improved since the DoW was written
 - GROMACS includes OpenMP
 - DALTON also has some OpenMP...?
 - DISCRETE has been rewritten

- **T6.1 Analysis and structure for efficient parallelization**
 - DALTON @ Lindgren (KTH, BSC)
 - DISCRETE @ {MN | Altix} (BSC)
 - GROMACS
 - @ CRAY (KTH, BSC)
 - @ {UVs | Altix 4700} (LRZ)
 - @ ICE clusters (UOXF)

- **T6.2 Multi-level/multi-scale parallelization (UOXF)**
 - GROMACS with MPI+OpenMP (UOXF, KTH)
 - DISCRETE with SMPSs (BSC)
 - (Later) DALTON with MPI+SMPSs (BSC, KTH)
- **T6.3 Ensemble computing techniques for scalability (KTH)**
 - GROMACS with COMPSs (BSC, KTH)
- **T6.4 Porting algorithms to accelerator architectures (SYN)**
 - DALTON (KTH, SYN) ???

... something else?

...should we do code parallelization? prototypes?

- **LRZ contribution**

LRZ will not do any code development, we will just do the analyses using Vampir tool for:

- *Gromacs with MPI on (SGI UV)*
- *Gromacs with MPI + OpenMP (SGI UV)*
- *And Testing Gromacs and Dalton on our new GPU cluster (CUDA)*

...Need to move effort between tasks???

What I would like.....

- From Code owners – how useful is the feedback we give you? How can be improved?
- From T6.2-T6.4 leaders – can you coordinate and complete the list of actions? How we are going to coordinate these actions with work within T6.1?

Inputs to WP6

- WP3 – suggest interesting analysis, relevant input cases for T6.1, *provide tracefiles*
- WP4 – may identify underperforming cases

Outputs from WP6

- WP2, WP5 – material about codes performance

