

MPI-multicore: Applications Requirements

Questionario Originale

	GAIA	Einstein-Tk	NEMO	NAMD	QuantumEpresso	RegCM
1	Code Developer - E.g.: P(=personal) ,OS(=OpenSource), C(=Commercial), ...					
	OS+P	OS+P	OS+P	OS	OS	OS
2	Parallelization Model - E.g.: MPI, openMP, Hybrid, GPU, ..					
	MPI/openMP	MPI/openMP	MPI/openMP	MPI/openMP	MPI/openMP GPU	MPI
3	CPU requirements - E.g.: 1-10 WholeNodes, 16-24 CPUs, ..					
	8-64 WholeNodes	1-64 WholeNodes	1 or more WholeNode Node	1-1024	8-128 WholeNodes	1 WholeNode
4	Memory requirements - E.g.: No, 1-2 GB per core, Memory-Bound(=whole avail. mem.), ..					
	Mem-bound	1GB per core	1GB per core	no	1-2 GB	No
5	Match Making - Yes(wms can find a suitable resource) , No(I select the resource)					
	No	No	No	Yes (no preinstalled exe)	No	Yes
6	Compiler/Version needed on the WN - E.g.: No=compiled on the UI, gcc/g++, icc, Java ..)					
	gcc-c++	f90, gcc-c++	NO	NO	No	No
7	Libraries/version needed on the WN (COMPILE time) - E.g.: no(=compiled on the UI), Blas, Lapack, Gsl, ..					
	cfitsio	blas, lapack, gsl, hdf5, fftw3	if compiled, netcdf	no	no	no
8	Libraries needed on the WN (EXECUTION time) - E.g.: Blas, Lapack, Gsl, ..					
	cfitsio	blas, lapack, gsl, hdf5, fftw3	no (netcdf statically linked)	no	no	no
9	Interpreter needed on the WN - E.g.: Python, perl, ..					
	no	no	Pyhton wrapper created	No	no	no
10	Applications needed on the WN - Name and version (if important) of a needed Application (QE, gaussian,..)					
	no	no	no	no	QE-latest-vers	no
11	Large amount of Data - E.g.: No, 10GB Input, 20-30 GB output, ...					
	400GB	20GB output	10GB input	10GB output	10 GB output	100GB
12	Data Intensive - E.g.: No(=don't care), SAN(=Shared High speed SAN), Local(=1 Local scratch disk per Node, ..)					
	No	SAN	No	No	SAN/Local	No, files are saved to custom storage via OpenDAP
13	Expected Execution time - E .g.: No=within a few hours, 24-48h, 72h or more,..					
	?	>3weeks	>72h	>3 weeks	72 or more	72 or more
14	Checkpoints - E.g.: No(=don't care) Yes(=I need a safe local storage area to save CheckPoints)					
	Yes on the same site	Yes	can continue on different sites	No, output is retrieved via SE	Yes, on the same site	No, files are saved to custom storage via OpenDAP

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15	Communication Intensive - E.g.: No (=don't care) , IB(=Infiniband needed) , ...					
	No	IB	No	IB if more than 3 physical nodes used	IB	no
16	Web portal - E.g.: No(not needed) , D(=yes for Data management) , CI (yes with Customized Interface), CHK=(Checkpoint support)...					
	CI	CI	CI	No	No	D
17	Main requirements and Expected outcomes (e.g.: optimized compilers/libraries, distributed File-systems, execution speedup, ..)					
	Application memory bound (up to 8TByte) - Typical resources are Supercomputers (Prace). Grid used for tests and small problems	Long term execution and large file produced (>10GB). Needed fast checkpoint area on dedicated sites.	Nemo needs standard HPC resources available on the Grid. The tool is statically compiled on the UI, so it doesn't need special SW env.	Long execution time, but we split in several small task with checkpointing. No special Sw env need so match-making can be used	Q/E needs to be installed (latest and optimized version) on the site. Low latency network and checkpoint needed	Standard execution requires large dataset and checkpoint, but REgCM relies on custom network storage systems (openDAP). The approach based on "relocatable package" (see appl. descriptions) makes the application suitable for the Grid Environment

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