

Computing requirements/scenarios

Table 1 – Proof-of-concept using CPUs (1st stage). Requirements/scenarios by priority.

Use Case	Number of CPU cores	RAM requirements per CPU core	Storage requirements	Inbound/Outbound during execution	Licensed software	Graphical interface	Operating System	Other Requirements
Molecular Dynamics simulations	24 to 48	512 Mb	150 Gb	No	No	No	Linux (Red Hat-based)	<ul style="list-style-type: none"> - SSH for access - Rsync for data transfer
Chemoinformatics applications/workflows	24 to 48	1 to 2 Gb	500 Gb	No	Yes	No	Linux (Red Hat-based)	<ul style="list-style-type: none"> - ORACLE JRE - OpenMPI v1.6 for distribution of processes across CPU cores - SSH for access - Rsync for data transfer
Third-party, licensed, Linux applications	4 to 8	1 Gb	50 Gb	Yes	Yes	Yes	Linux (Red Hat-based and Ubuntu LTS)	<ul style="list-style-type: none"> - SSH for access - Rsync for data transfer - FlexLM license server - VNC or NoMachine Server for access?
Third-party, licensed, Windows applications	4 to 8	1 Gb	50 Gb	No	Yes	Yes	Windows (Windows 7, Windows 8)	<ul style="list-style-type: none"> - Remote Desktop for access?

Table 2 – Proof-of-concept using GPUs (2nd stage). Requirements/scenarios by priority.

Use Case	CPU/GPU	RAM requirements per CPU core	Storage requirements	Inbound/Outbound during execution	Licensed software	Graphical interface	Operating System	Other Requirements
Molecular Dynamics simulations	8-12 CPU cores per GPU 1 to 4 GPUs	1Gb	150 Gb	No	No	No	Linux (Red Hat-based)	<ul style="list-style-type: none"> - SSH for access - Rsync for data transfer
Cheminformatics applications/workflows	4 CPU cores per GPU 1 to 4 (high-mem) GPUs	1 to 2 Gb	750 Gb	No	Yes	No	Linux (Red Hat-based)	<ul style="list-style-type: none"> - ORACLE Java Runtime Environment - SSH for access - Rsync for data transfer