HPC/HTC Workflows for the Computational Chemistry Community

XSEDE-EGI Collaborative Use Examples

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Background

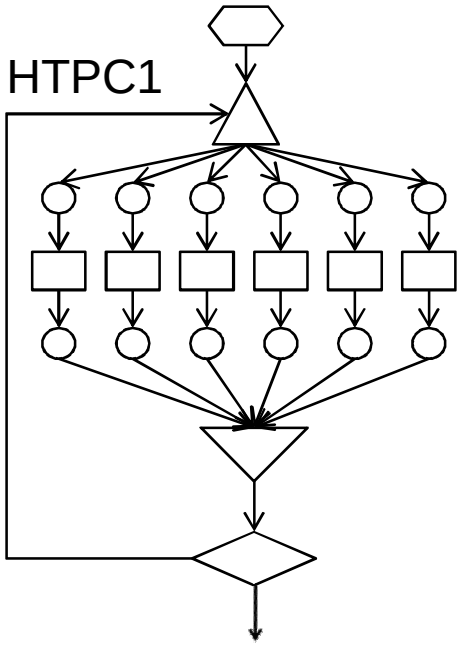
- The Chemistry and Molecular and Materials Science and Technology (CMMST) community
  - is developing a set of activities aimed at equipping its applications with a set of tools facilitating interoperability between HPC and HTC platforms
  - is developing tools that act as a unique point of access to the different infrastructures (portals, GUIs, etc)
  - is operatively supported in EGI by the COMPCHEM VO and there is a cooperation agreement aimed at supporting the VO in OSG
  - is running a VT in order to establish a CMMST Virtual Research Community
  - is involving US collaborators in the VT

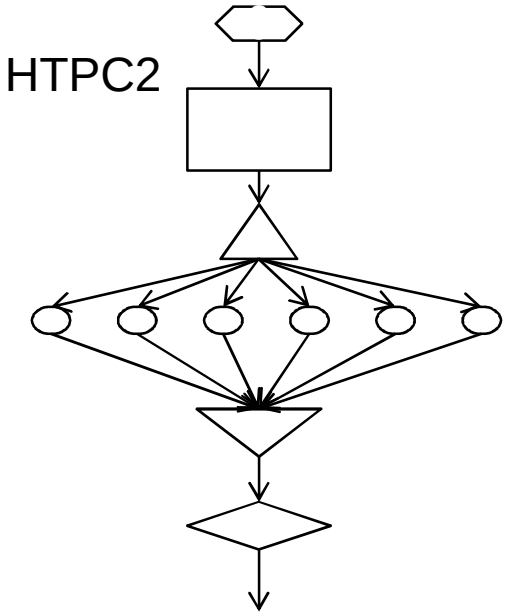
Communities involved

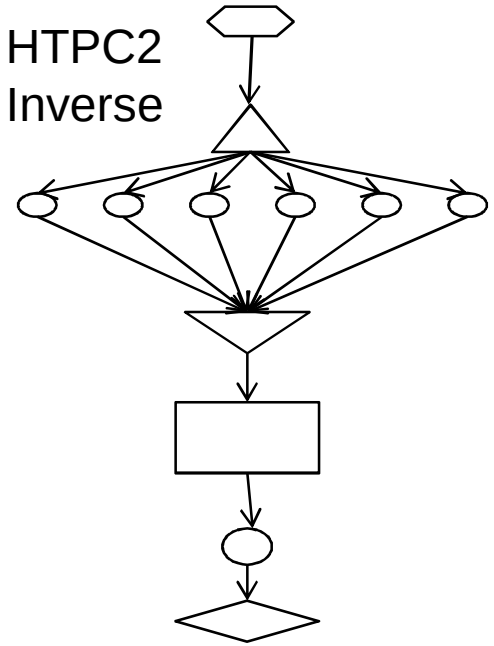
- To implement these activities the CMMST Community is collaborating with several actors both in Europe and US:
  - On the European side with the COMPCHEM VO supported by several NGIs and with EGI.eu
  - On the US side the with the High Performance Computing Center and the Chemical Dynamics group of the Department of Chemistry and Biochemistry both at the Tech University of Texas (Lubbock) of which the latter is:
    - specialized in classical, semi-classical, and quantum mechanical methods applied to chemical reactions at an atomistic level
    - Developer of the VENUS general chemical dynamics computer program

- A set of real life use cases requiring mixed HPC/HTC workflows were selected within the community
  - Grouped into prototypical workflows (HTPC skeletons)
  - Involving commonly used applications

HTPC Skeletons







Within the EGI-XSEDE collaboration we would like to perform a feasibility study on running real life use cases based on these HTPC skeletons by exploiting the two infrastructures

- in an automated minimizing the human intervention
- possibly developing prototypical tools able to handle the skeletons (in both the computing and data management parts).

HPC run

Scalar or small parallel run

Selected use cases

a) Exact quantum dynamics calculations for Li + FH (HTPC2)
b) Exact dynamics of nuclear and electronic systems within cavities (HTPC2)
c) Ab initio calculations for N_2 + N_2 system (HTPC1)
d) Molecular Dynamics simulations of Carbon NanoTubes (HTPC1)
e) Ab initio and classical Molecular Dynamic simulations in micropourus materials (HTPC2)
f) Interactions between doxorubicine and γ-cyclodextrin (HTPC1)
g) Semiclassical simulations of spectroscopy (HTPC2 inverse)

Computational Requirements

Application	HPC requirements			HTC requirements		
	Cores /job	Memory (GB/core)	Total allocated time (h)	Cores /job	Memory (GB/core)	Total allocated time (h)
ABC (use case a)	32	2	25k	1	2	50k
MCTDH (use case b)	1	10	50k	5	1	40k
GAMESS-US (use case c)	32	2	300k			
DL_POLY (use case d)	64	2	100k	8	1	500k
CP2K (use case e – HPC)	512	2	512k			
NAMD (use case e – HTC)				8	1	40k
NAMD (use case f)	256	1	50k	32	1	60k
SC-IVR (use case g)	16	2	50k	1	2	50k

No particular data requirements – few GB per run at maximum

X509 access (GT on the XSEDE resources: gsi-ssh, globus-url-copy, etc)

Use cases provided by...

- **William L Hase / Alan Sill**

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HPC Center

Texas Tech University

- **Sergio Rampino**

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INFN-IGI – Italian NGI user support team