



# Ohio Supercomputer Center

An **OH·TECH** Consortium Member

## SUG Software Committee Report

Rick Prairie  
Apr 5, 2017

Attendees: Richard Prairie, Tom Beck, Heechang Na, and David Hudak



# Call for Participation

- When
  - Software committee meets prior to SUG meetings
  - Discussion via email between meetings
- What
  - Decisions on which software packages are purchased for academic use, respond to new software requests





# Recent/Upcoming Decisions

- **New Purchase Discussion**
  - Comsol Server: provide non-OSU users
  - Debugger: Totalview vs. DDT
- **Third party hosting**
  - Matlab
    - Any academic users in Ohio can use Matlab on OSC as part of our license.
- **Discontinue?**
  - CSD (Cambridge Structural Database)
    - Not HPC software
- **Capital purchase**
  - Intel Parallel Studio Cluster Edition (Done)
  - Totalview (Sep 28, 2017)
  - Ansys (Nov 8, 2017)



## Renewals/Purchases – Since Oct. 2016 meeting

Software	Expiration/ option	License Term	Cost	Renewal Status
Abaqus	Oct 31, 2016	1	\$16,826.55	Done
pgi	Dec 5, 2016	1	\$2,980	Done
CSD	Dec 31, 2016	1	\$2,640	Done
Gaussian	Dec 31, 2016	1	\$12,000*	Done
Intel Cluster	Jan 30, 2017	5	\$25,226.25	Done
MDCS (OSU)	Feb 28, 2017	1	\$588.80	Done
MDCS (non-OSU)	Mar 31, 2017	1	\$1,472	Done
Turbomole	Apr 28, 2017	1	\$2,616	Done

\* Contribution from user for portion of the cost



## Pending/Upcoming Purchases – until Dec. 2017

Software	Expiration/option	License Term	Projected Cost	Renewal Status
Amber	New version	perpetual	\$2,000	
Comsol	Jun 30, 2017	1	\$8,221	
Comsol server	New purchase	1		
Q-chem	Sep 13, 2017	1	\$4,100	
Star-CCM+	Sep 23, 2017	1	\$5,000	
Totalview	Sep 28, 2017	5	\$31,588	DDT?
Schrodinger	Oct 13, 2017	1	\$8,850*	
Allinea	Oct 14, 2017	1	\$4,776	DDT?
abaqus	Oct 31, 2017	1	\$16,826.55	
Ansys	Nov 8, 2017	5	\$141,996.25	
pgi	Dec 5, 2017	1	\$2,980	
Gaussian	Dec 31, 2017	1	\$12,000*	

\* Contribution from user for portion of the cost





# Summary

- **New Purchase Discussion**
  - Comsol Server: provide non-OSU users
  - Debugger: Totalview vs. DDT
- **Third party hosting**
  - Matlab
    - Any academic users in Ohio can use Matlab on OSC as part of our license.
- **Renewal (Since Oct 2016 meeting)**
  - Abaqus, pgi, CSD, Gaussian, Intel Cluster (Capital), MDCS, Turbomole
- **Upcoming (during 2017 calendar year)**
  - Discontinue?: CSD (Cambridge Structural Database)
  - Capital purchase: Totalview, Ansys
  - Regular renewal: Amber, Comsol, Q-chem, Star-CCM+, Schrodinger, Alinea, abaqus, pgi, Gaussian

