# Introduction to the licensed software portfolio

*Attila Fekete*
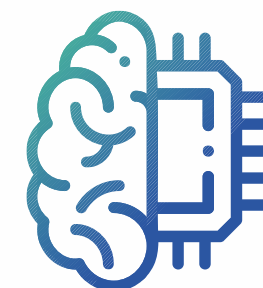
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# Currently on-going procurements

- Ansys
- Amber 22
- SCM – Amsterdam Density Functional
- CHARMM
- Gaussian 16

- Schrödinger Suite
- TeraChem
- Intel oneAPI HPC Toolkit
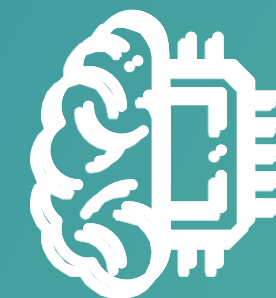- Matlab (through academic agreements)

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# Ansys

- Advanced engineering simulations
- 3D design, materials, structures
- Autonomous Vehicle Simulation
- Electronics, Optics, Photonics, Semiconductors
- Fluids (CFD simulations)
- License for 3 years – 256 core workgroup
- 25 research and 250 educational license

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# Amber22

- „Fastest academic GPU MD simulation engine"
- High level GPU utilization by pmemd (Legrand & Walker)
- Advanced MD software for PB macromolecular simulations
- Extensive analysis tools
- Interfaces for many other softwares
- Perpetual license



Amber 2022
Reference Manual
(Covers Amber22 and AmberTools22)

# ADF (AMS2022)

- „Fast and accurate density functional calculations"

- ADF – DFT program for molecules, spectroscopy, inorganic chemistry
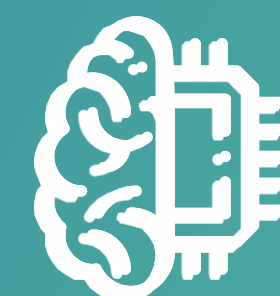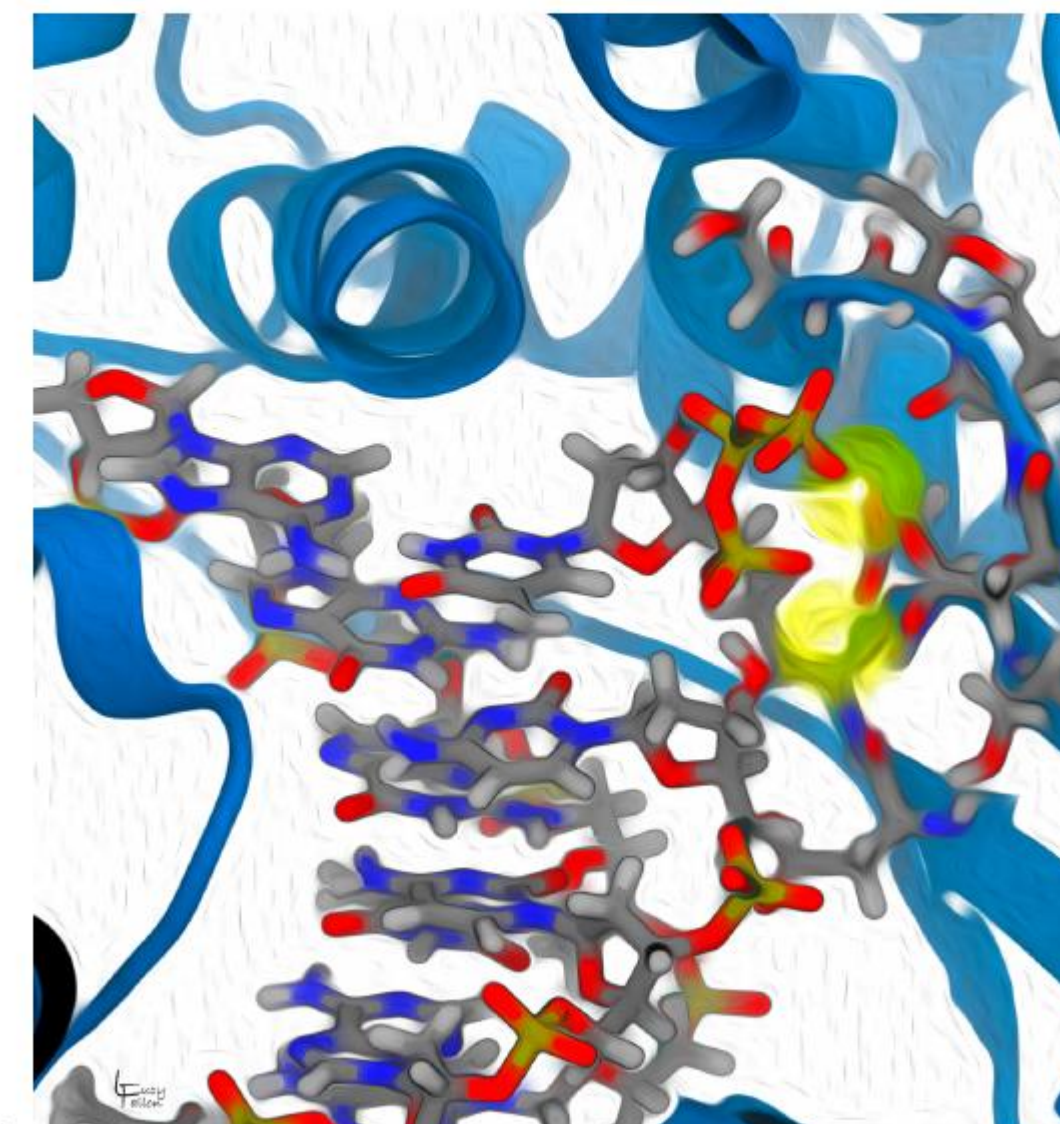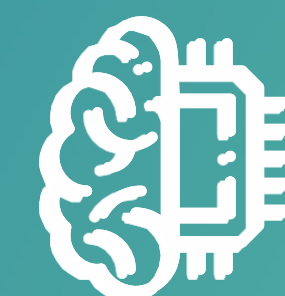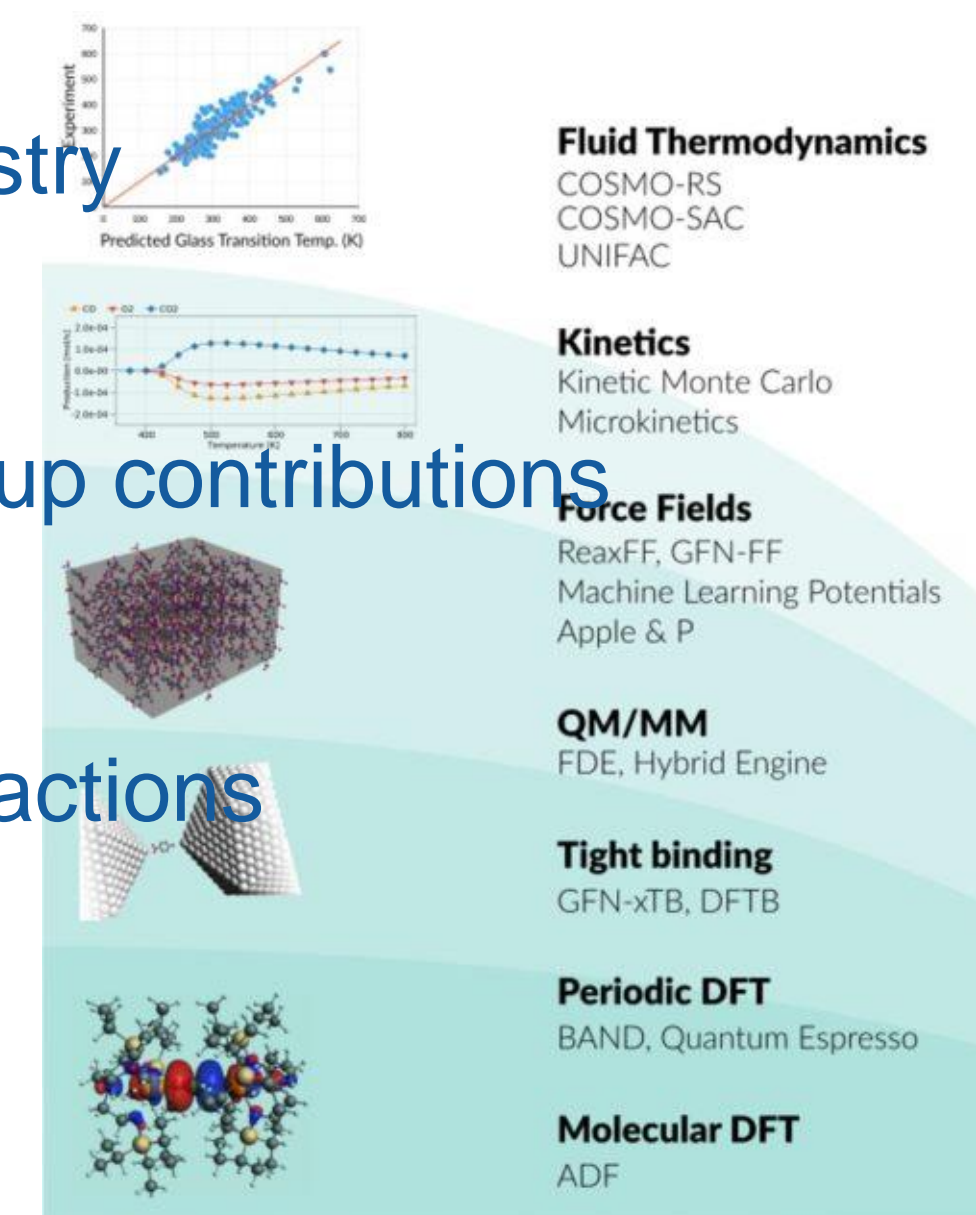
- BAND – periodic DFT for condensed matter, incl. bulk, surfaces

- COSMO-RS – fluid thermodynamics, property predictions from group contributions

- DFTB – DF Tight Binding, fast approximate DFT for 1D, 2D, 3D

- ReaxFF – Reactive FF for large-scale MD simulations w/chem. Reactions

- MLPlot – Machine Learning Potential backend for PES tasks

- 3-year „old-style" full bundle for unlimited cores incl. new releases



**Fluid Thermodynamics**
COSMO-RS
COSMO-SAC
UNIFAC

**Kinetics**
Kinetic Monte Carlo
Microkinetics

**Force Fields**
ReaxFF, GFN-FF
Machine Learning Potentials
Apple & P

**QM/MM**
FDE, Hybrid Engine

**Tight binding**
GFN-xTB, DFTB

**Periodic DFT**
BAND, Quantum Espresso

**Molecular DFT**
ADF

# CHARMM

- Swiss army-knife of MD suites, led by Martin Karplus
- Enhanced sampling methods
- Multi-scale techniques (QM/MM, MM/CG)
- Simulations of biological systems in solution, crystal and membrane
- Analysis and model building tools
- Parallel cluster and GPU support
- Perpetual license
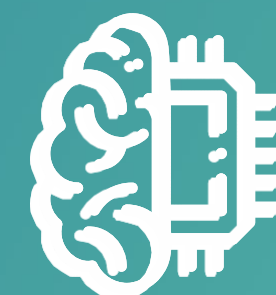


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# Gaussian16


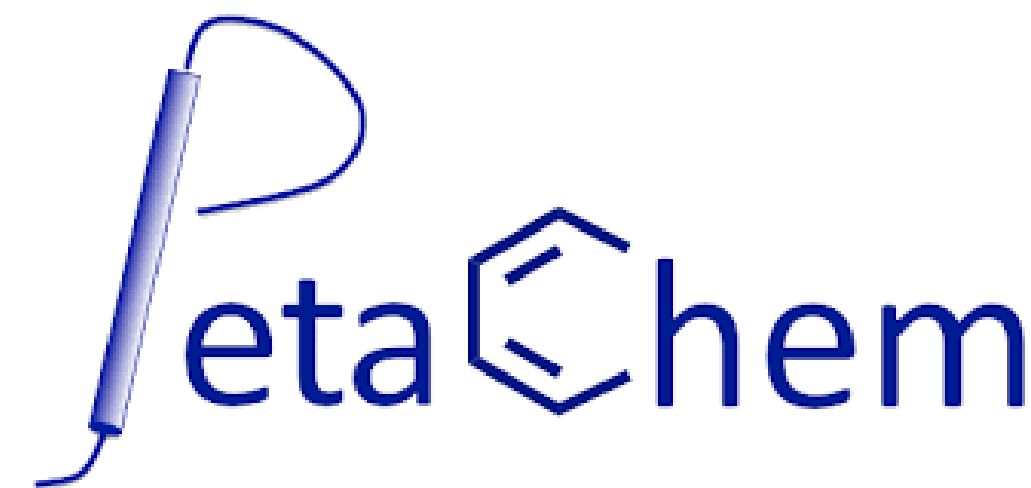*Expanding the limits of computational chemistry*

- The most cited quantum chemistry software
- Easy to use & robust
- Hartree-Fock, (TD-)DFT, post-HF & semiempirical methods
- Solvation models, spectroscopy
- Hybrid methods by ONIOM (QM/QM, QM/MM, QM/QM/MM)
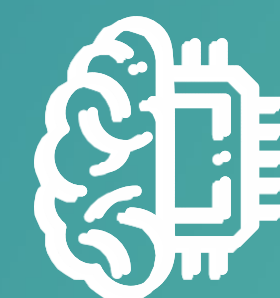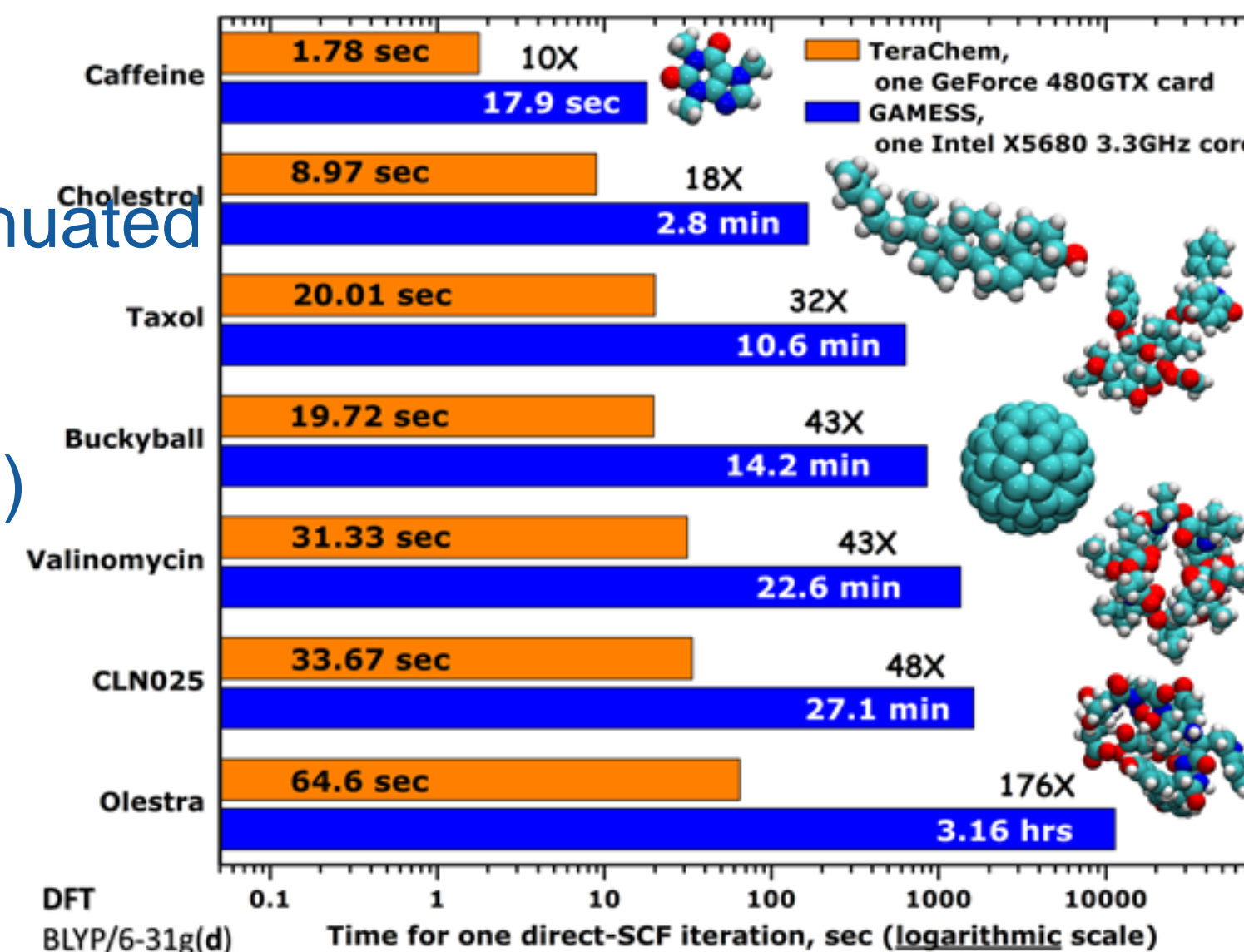- Partial GPU support
- Perpetual license
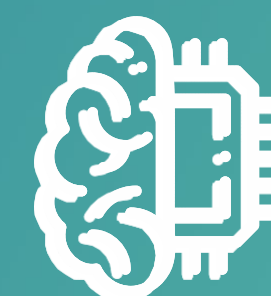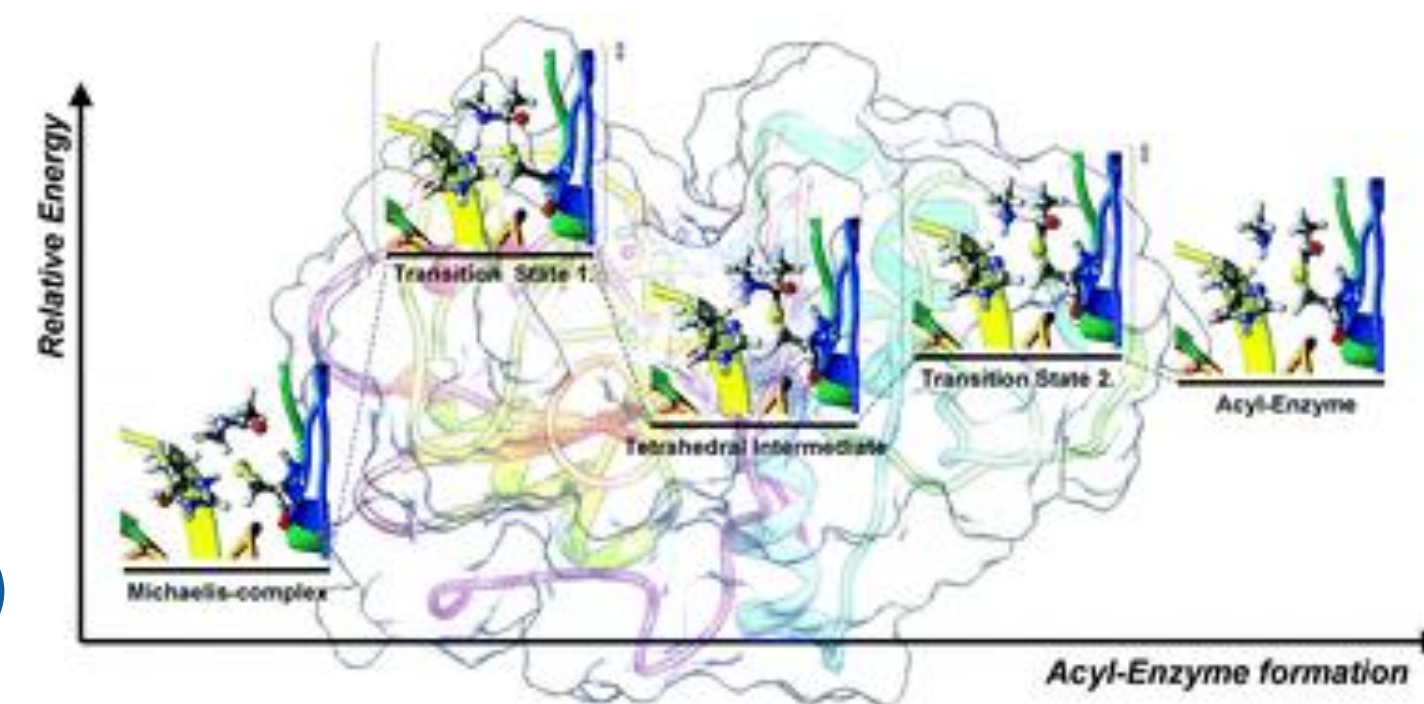
# TeraChem



- General purpose QC software designed to run on nVidia GPUs
- HF & grid-based Kohn-Sham energy and gradient calcs.
- Various DFTs, incl. long-range corrected & Coulomb attenuated
- TD-DFT and CIS
- Geometry optimizations (L-BFGS, conjugate gradient, SD)
- Ab initio MD (NVE, NVT ensembles)
- Multi-GPU support, single/dynamic/double precision
- 1-year license



| | | |
|---|---|---|
| Caffeine | 1.78 sec | 10X |
| | 17.9 sec | |
| Cholestrol | 8.97 sec | 18X |
| | 2.8 min | |
| Taxol | 20.01 sec | 32X |
| | 10.6 min | |
| Buckyball | 19.72 sec | 43X |
| | 14.2 min | |
| Valinomycin | 31.33 sec | 43X |
| | 22.6 min | |
| CLN025 | 33.67 sec | 48X |
| | 27.1 min | |
| Olestra | 64.6 sec | 176X |
| | 3.16 hrs | |

TeraChem, one GeForce 480GTX card
GAMESS, one Intel X5680 3.3GHz core

DFT BLYP/6-31g(d)

Time for one direct-SCF iteration, sec (logarithmic scale)

# Schrödinger suite

- From drug discovery to material science and for everything in between

- Interchangeable token library (50 tokens)

- Basic - AutoQSAR, MacroModel, Epik, Jaguar, Canvas, Qsite

- Ligand- & structure-based – (Phase, Shape screening, Field-based QSAR,

- Glide, Prime, Core hopping, Prime X

- Desmond GPU – 10 floating liceneses

- OPLS FF – 1 access license

- Add-on floating licenses (20) – Glide, Prime, Phase, Jaguar, QSite

- 3-year license for academic use
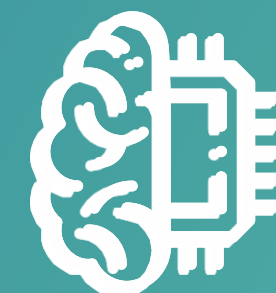
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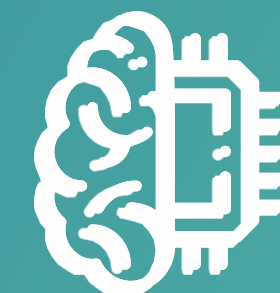
# Intel oneAPI HPC Toolkit

- DPC++/C++ compiler
- C++ compiler classic
- Cluster checker
- Fortran compiler
- Intel Inspector
- MPI library
- Trace analyzer & collector
- 2 concurrent user, multi-node – 3-year

intel

1

oneAPI

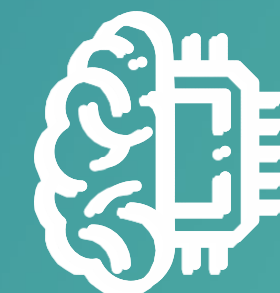HPC TOOLKIT

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# TotalView

- The most advanced debugger for HPC

- Simplify HPC debugging

- Streamline GPU debugging

- Improve insight and control

- Increase efficiency

- Debug code in multiple languages

- Simplify new platform adoption

- 3-year license, 8 token
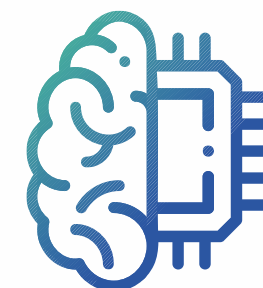
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# Matlab
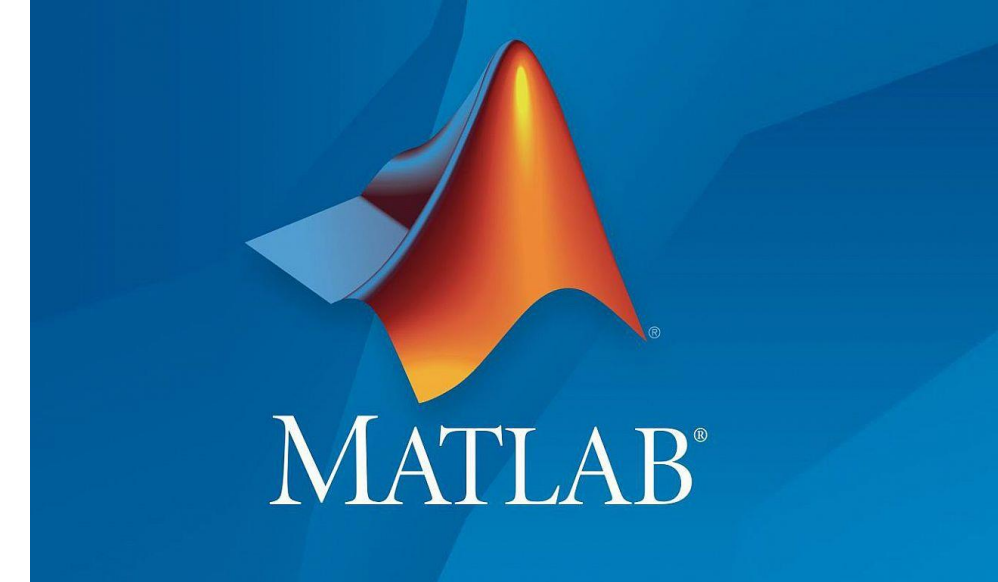
- Through hosting provider agreements with universities

- Data analysis, Graphics (data visualization)

- Programming

- App building & external language interfaces

- Hardware and parallel computing
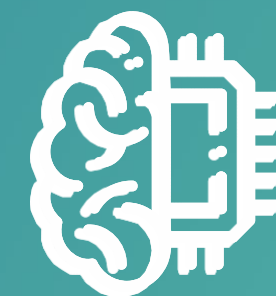
# Thanks
# for your attention!

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