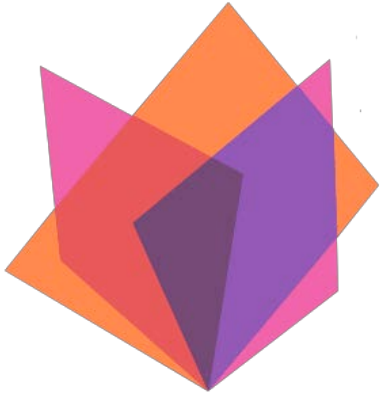
OpenMP®

SC'20 Booth Talk Series



OpenMP Use Cases

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Automotive	Speed up mapping for autonomous driving	Autoware
Financial	Speed up European Option Pricing	Black-Sholes
Physics	Simulate processes of high-energy density physics	HYDRA

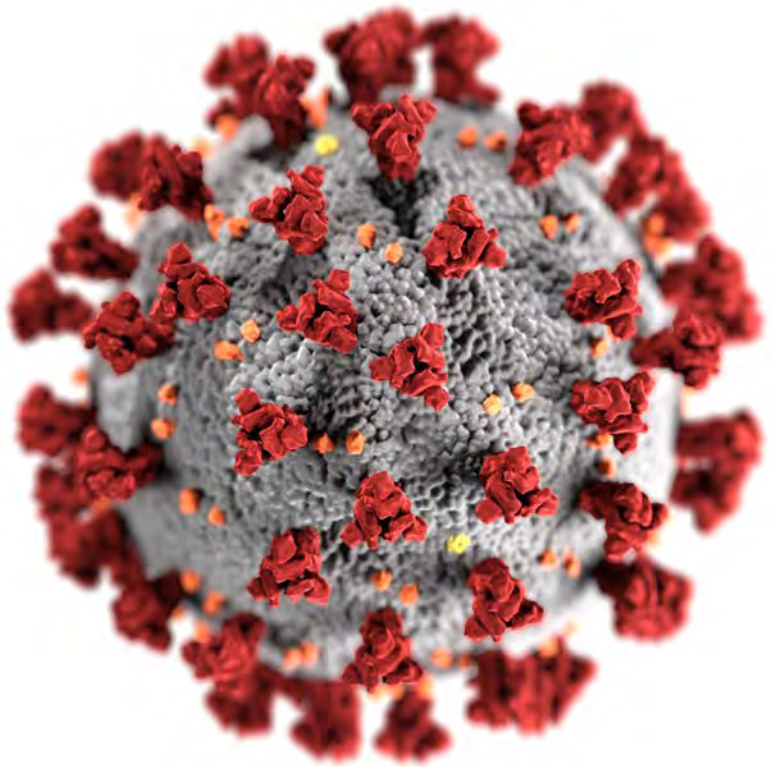
Speed up Search for COVID-19 Drug

AutoDock is a molecular docking application, used for searching COVID-19 drug candidates

The Lamarckian Genetic Algorithm is the compute intensive part

The LGA was parallelised with hybrid OpenMP/MPI

AutoDock is used a.o. on MOGON II, the Mainz supercomputer system



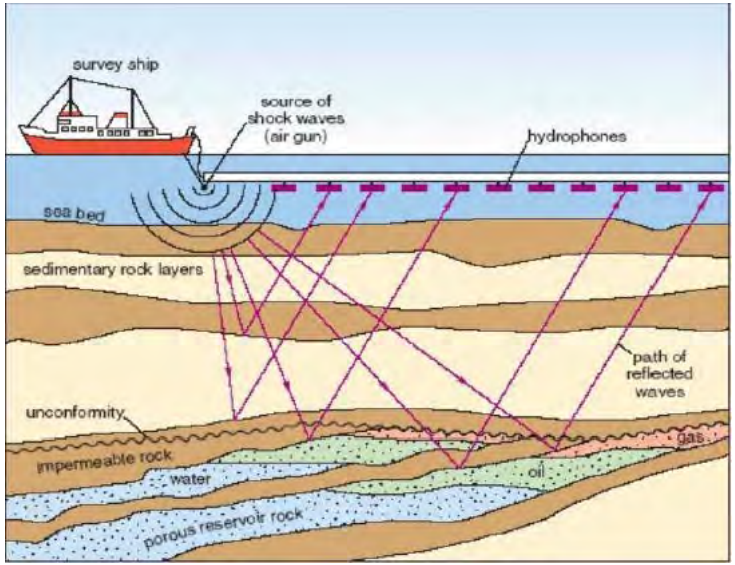
Speed up Seismic Analysis

Minimod is a stencil-based application that solves the wave equation

Computational intensive part is stencil computation

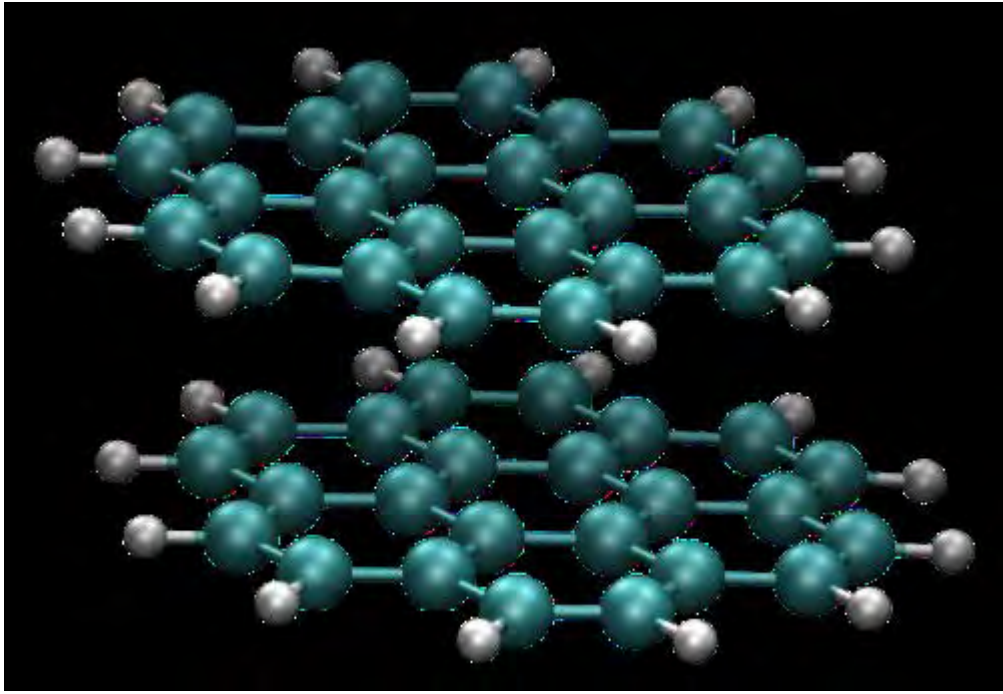
Implemented with OpenMP tasks

Used by TOTAL & Stony Brook University on Summit and Cori



Compute Binding Energy of the Coronene Dimer

- NWChem is a widely used Open Source package for Computational Chemistry
- Quantum mechanical computations are compute intensive
- The intra-node and accelerator offload features of OpenMP 4.5 are used.
- Widely used and available on many HPC systems incl Shaheen, Cori …



Coronene Dimer

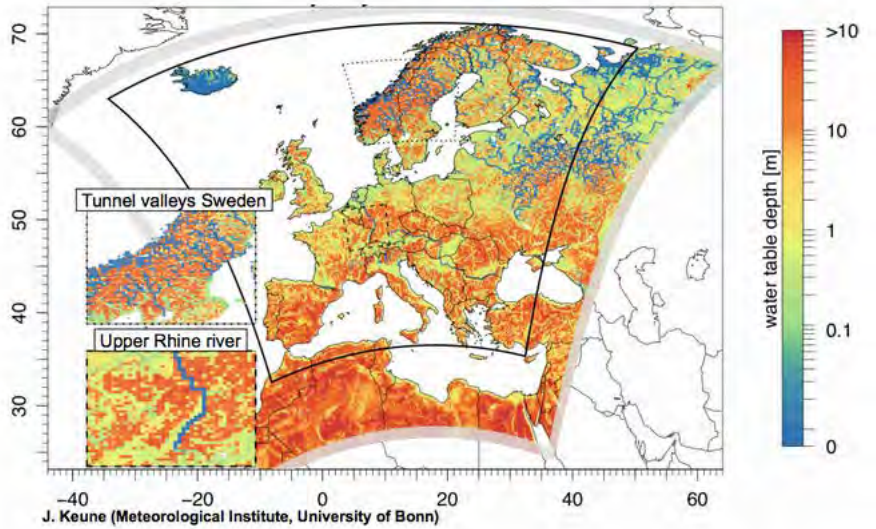
Speed up Modelling of Surface and Subsurface Flow

ParFlow is a watershed model to simulate surface and subsurface fluid flow.

Computational intensive non-linear and multigrid solvers, and coupled land-water models.

OpenMP is back end for intra-node parallelism

Used on up to 30K processors on supercomputers such as Edison, Cori, Yellowstone, & JUQUEEN

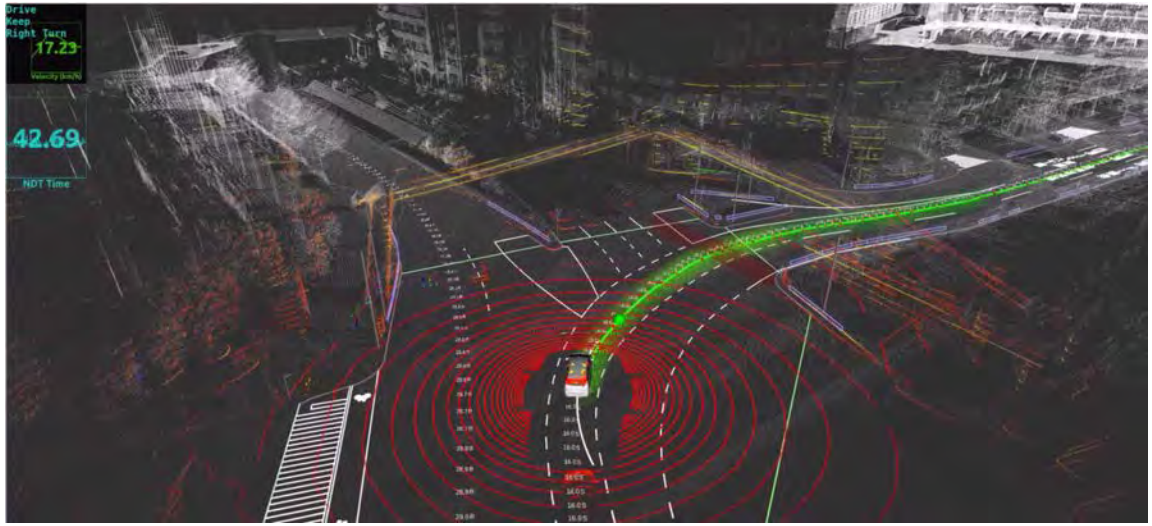


Groundwater-land surface-atmosphere feedbacks during the European 2003 heat wave

Speed up Mapping for Autonomous Driving

Software is the Autoware Autonomous Driving Platform

Mapping module is computational intensive



Implemented with OpenMP device offloading and parallelization directives

Target platforms are Nvidia GPU and Renesas R-Car processors

Speed up European Option Pricing

- Solve the Black-Scholes PDEs
- Embarrassingly parallel problem, no data dependences
- Parallelised with OMP PARALLEL
- Implemented on shared memory systems

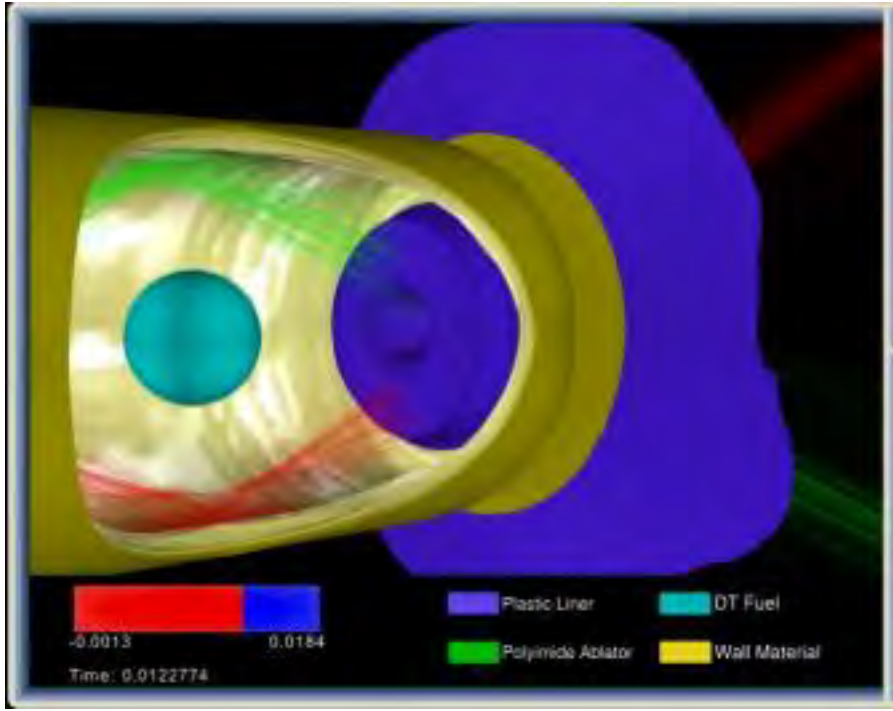
Simulate the Processes of High-Energy Density Physics

HYDRA is a multi-physics simulation code to simulate radiation transfer, atomic physics, & laser propagation

Quantum mechanical computations are compute- intensive.

Implemented with hybrid OpenMP/MPI

Developed and used by LLNL to simulate fusion and nuclear processes



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