

# HPC beyond R&I

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HPC enables organizations to tackle problems that are computationally infeasible otherwise, leading to faster innovation, better risk management, and significant cost savings.

## HPC Use Cases by Industry

Industry	Business Unit/Area	Discipline & Description	Technique/Algorithm	Computing Complexity	Problem to Solve	Business Impact	HPC Value Proposition
Pharmaceuticals	Drug Discovery	Computational Chemistry, Molecular Dynamics, Structure-based Drug Design	Molecular Dynamics (MD), Quantum Chemistry (DFT), Docking	High	Predicting drug-target interactions, optimizing leads	Faster drug development, reduced R&D costs	Enables simulation of large biomolecules, accelerates virtual screening
Automotive	Engineering /Design	Crash Simulation, Aerodynamics, Materials Modeling	Finite Element Analysis (FEA), Computational Fluid Dynamics (CFD)	High	Vehicle safety, fuel efficiency, material optimization	Improved safety, lighter vehicles, faster prototyping	Allows detailed, multi-physics simulations, reduces physical testing
Energy	Exploration /Production	Seismic Imaging, Reservoir Simulation	Reverse Time Migration (RTM), Full Waveform Inversion (FWI), Reservoir Modeling	Very High	Locating oil/gas reserves, optimizing extraction	Higher yield, reduced exploration risk	Processes massive geophysical datasets, improves accuracy
Manufacturing	Process Optimization	Digital Twins, Predictive Maintenance	Machine Learning (ML), Physics-based Simulation	Medium-High	Equipment failure prediction, process efficiency	Reduced downtime, increased productivity	Real-time analytics, large-scale simulation capability
Finance	Risk Analysis	Quantitative Modeling, Portfolio Optimization	Monte Carlo Simulation, Option Pricing (Black-Scholes, Heston)	High	Market risk assessment, pricing complex derivatives	Better risk management, competitive advantage	Enables millions of simulations in parallel, faster decision-making
Aerospace	Design /Testing	Aerodynamics, Structural Analysis	CFD, FEA, Multidisciplinary Optimization	High	Aircraft performance, structural integrity	Safer, more efficient aircraft, reduced time-to-market	Simulates complex systems, integrates multiple physics domains
Weather /Climate	Forecasting	Climate Modeling, Weather Prediction	Numerical Weather Prediction (NWP), Ensemble Forecasting	Very High	Accurate weather /climate forecasts	Disaster preparedness, agricultural planning	Processes global-scale models, improves forecast resolution
Life Sciences	Genomics	DNA Sequencing, Population Genomics	Sequence Alignment (BLAST, BWA), Genome Assembly	High	Analyzing large genomic datasets, variant detection	Personalized medicine, disease research	Handles petabyte-scale data, accelerates analysis
Chemicals	Materials Discovery	Polymer Modeling, Reaction Kinetics	Molecular Dynamics, Quantum Chemistry, ML	High	New material discovery, reaction optimization	Faster innovation, reduced experimental costs	Simulates complex chemical systems, supports AI-driven discovery

### Pharmaceuticals: Drug Discovery

- Discipline: Computational Chemistry, Molecular Modeling
- Techniques: MD, DFT, Docking
- Complexity: High (large biomolecules, long timescales)
- Problem: Predicting drug efficacy and safety before synthesis
- Business Impact: Accelerates drug pipeline, reduces costs
- HPC Value: Enables virtual screening of millions of compounds

### Automotive: Crash Simulation & Aerodynamics

- Discipline: Engineering Simulation

- Techniques: FEA, CFD
- Complexity: High (multi-physics, fine mesh)
- Problem: Ensuring safety and efficiency
- Business Impact: Reduces prototyping costs, improves safety
- HPC Value: Allows detailed, rapid simulation of full vehicles

## Energy: Seismic Imaging & Reservoir Simulation

- Discipline: Geophysics, Reservoir Engineering
- Techniques: RTM, FWI, Reservoir Modeling
- Complexity: Very High (large 3D datasets)
- Problem: Locating and extracting resources efficiently
- Business Impact: Increases yield, reduces risk
- HPC Value: Processes massive datasets, improves subsurface imaging

## Manufacturing: Digital Twins & Predictive Maintenance

- Discipline: Industrial Engineering, Data Science
- Techniques: ML, Physics-based Simulation
- Complexity: Medium-High
- Problem: Predicting failures, optimizing processes
- Business Impact: Reduces downtime, increases throughput
- HPC Value: Real-time analytics, large-scale simulation

## Finance: Risk Analysis & Portfolio Optimization

- Discipline: Quantitative Finance
- Techniques: Monte Carlo, Option Pricing Models
- Complexity: High (many scenarios, real-time)
- Problem: Assessing risk, pricing derivatives
- Business Impact: Better risk management, faster trading
- HPC Value: Enables parallel simulation of millions of scenarios

## Aerospace: Aerodynamics & Structural Analysis

- Discipline: Aerospace Engineering
- Techniques: CFD, FEA, Optimization
- Complexity: High (multi-disciplinary)
- Problem: Optimizing performance and safety
- Business Impact: Faster design cycles, safer aircraft
- HPC Value: Integrates multiple physics, accelerates design

## Weather/Climate: Forecasting & Modeling

- Discipline: Meteorology, Climate Science
- Techniques: NWP, Ensemble Forecasting
- Complexity: Very High (global models)
- Problem: Accurate, timely forecasts
- Business Impact: Disaster mitigation, planning
- HPC Value: Higher resolution, more accurate predictions

## Life Sciences: Genomics

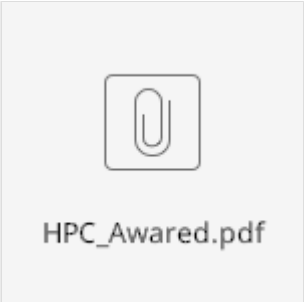
- Discipline: Bioinformatics
- Techniques: Sequence Alignment, Genome Assembly
- Complexity: High (petabyte-scale data)
- Problem: Fast, accurate genome analysis
- Business Impact: Personalized medicine, research
- HPC Value: Accelerates analysis, enables population-scale studies

## Chemicals: Materials Discovery

- Discipline: Computational Chemistry, Materials Science
- Techniques: MD, Quantum Chemistry, ML
- Complexity: High
- Problem: Discovering new materials, optimizing reactions
- Business Impact: Faster innovation, cost savings
- HPC Value: Simulates complex systems, supports AI-driven discover

## Benchmarks

References



HPCwire Readers' Choice Awards 2025