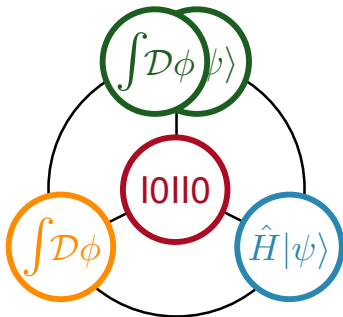# Profiling and Optimizing ORCA:
Overcoming Challenges in Complex Quantum Chemistry Codes

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Outline

- Introduction: The ORCA Package and HPC Challenges
- A Multi-Tool Strategy for Performance Analysis
- Uncovering issues and Collaborative Development
- Future Directions

ORCA: A Quantum Chemistry Package with HPC Challenges

- **ORCA**: Widely-used quantum chemistry package
- Code generated automatically: (ORCA AGE)
- Focus on Coupled Cluster: CCSD(T)
- **Challenge**: Complex execution model makes profiling and optimization difficult
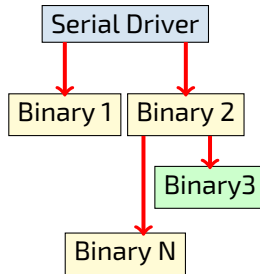
Objective: Profile, analyze, and optimize this complex application

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ORCA Profiling: From Challenge to Solution

The Challenge

- Driver launches binaries via `system` library
- Dynamic execution paths & separate build trees
- I/O bound computations
- Unnamed scopes → No symbol resolution
- Process pinning challenging
- Large code base

Standard profiling tools are insufficient

Our Solution: Tool Combination

- **Score-P**: Profile each binary
- **llview**: Monitor launch patterns
- **numactl**: Process pinning enforcement
- **Darshan**: I/O profiling

Score-P → ORCA ← numactl
llview → ORCA ← Darshan ↑
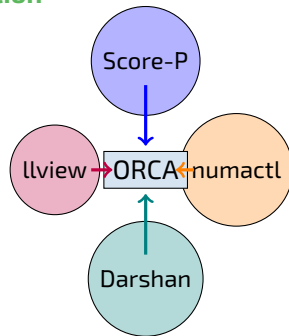
Specialized tools are required for complex execution models

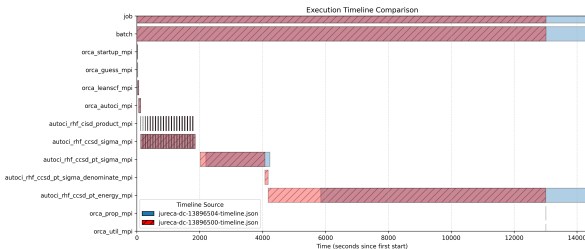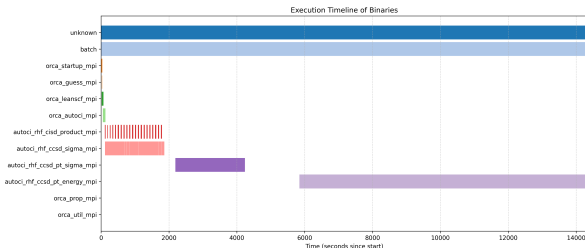⟨NuMeriQS⟩

Collaborative Optimization: Hidden gaps

Collaboratiion Results:

- Characterize execution patterns

- Identified gaps processes

- Developers implemented parallel processes

- API compatibility maintained

Quantified Benefits:

- Visible runtime reduction

- Better resource utilization

Execution Timeline of Binaries

Execution Timeline Comparison

Future Optimization Opportunities

Short-term Possibilities:

- Additional tensor contraction patterns
- Profiling code generation ORCA–AGE

Long-term Challenges:

- I/O improvements/ MPI-IO migration
- Execution model redesign
- Memory management improvements

What We've Learned:

- Profile ORCA it is very difficult: Single tool doesn't exist
- Takes substantial time and effort
- Close collaboration it is necessary
- Methodology is transferable to other ORCA's algorithms
- Complex codes can be systematically optimized

Ready for new challenges

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Questions?

Numeriqs Project Z02

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