Contribution ID: **431** Type: **Talk**

From Punch Cards to AI-Powered HPC: A 40-Year Journey in Computational Chemistry Infrastructure

Tuesday, 2 December 2025 13:30 (20 minutes)

This presentation chronicles the journey of an older-generation computational chemist and a young HPC expert, mediated via AI assistance, culminating in the successful deployment of a multi-node research computing cluster. The cluster supports molecular modeling and drug design, enabling large-scale molecular dynamics and quantum chemistry calculations. The senior researcher's four-decade arc—from 1983 punch cards to 2025 AI-collaborative infrastructure—illuminates artificial intelligence's role in transforming scientific knowledge transfer.

An initial Gaussian software request expanded into comprehensive cluster setup: Rocky Linux 9, Slurm management, parallel filesystems, and seven key packages (Gaussian, ORCA, GAMESS-US, Psi4, NWChem, CP2K and AMBER). This optimized mixed GPU architectures (RTX A4000/RTX 4060) — a common reality in most laboratories (perhaps fortunately for the average researcher), though uniform hardware is preferable if affordable. Benchmarks yielded 85% parallel efficiency, affirming production readiness.

The AI approach thrived despite hands-off administration, via an iterative model of problem-solving, explanation, and reasoning. Complementary tools — Claude AI for documentation, Grok for perspectives, DeepSeek for verification — fostered rapid consensus, with human-led execution, validation, and adaptation essential. This erodes barriers to retraining or consultancy, enabling expertise assimilation for resource-limited institutions and heralding a paradigm shift in scientific knowledge application.

Keywords: High-Performance Computing, Computational Chemistry, AI-Assisted Infrastructure, Cluster Computing, Knowledge Transfer, Slurm Workload Manager, Scientific Computing, Human-AI Collaboration, HPC Democratization, Intergenerational Learning.

Presenting Author

Yes

Email

Student or Postdoc?

Institute

Registered for the conference?

CHPC User

Yes

CHPC Research Programme

Workshop Duration

Primary author: Prof. GOVENDER, Krishna (University of Johannesburg)

Presenters: Prof. GOVENDER, Krishna (University of Johannesburg); KRUGER, Hendrick (UKZN)

Session Classification: HPC Applications

Track Classification: Computational Chemistry