**HPC Cluster for Amber (Molecular Dynamics)**

**🛠️ Hardware Selection:**

| **Component** | **Model** | **Qty** | **Unit Price (USD)** | **Total (USD)** | **Total (ZAR)** |
| --- | --- | --- | --- | --- | --- |
| **Compute Nodes** | HPE ProLiant DL385 Gen11 (AMD EPYC 9654, 96C/192T) | 2 | $6,500 | $13,000 | R260,000 |
| **GPUs** | NVIDIA RTX A6000 48GB | 2 | $2,500 | $5,000 | R100,000 |
| **Memory** | 256GB DDR5 ECC (per node) | 2 | $1,200 | $2,400 | R48,000 |
| **Storage** | 2TB NVMe SSD (per node) | 2 | $250 | $500 | R10,000 |
| **Networking** | 100Gbps Infiniband | 2 | $800 | $1,600 | R32,000 |
| **Switch** | 100Gbps Infiniband Switch | 1 | $3,000 | $3,000 | R60,000 |
| **Total** |  |  |  | **$20,000** | **R400,000** |

🔹 **Justification:**

* **Amber is FP64-heavy**, making **AMD EPYC 9654 (96 cores)** the best choice for **parallel molecular simulations**.
* **RTX A6000 (48GB VRAM)** provides a balance between high **double-precision performance** and **CUDA acceleration** for Amber.
* **100Gbps Infiniband ensures fast inter-node communication** for large-scale simulations.

**HPC Cluster for ICON (Weather Simulation)**

**🛠️ Hardware Selection:**

| **Component** | **Model** | **Qty** | **Unit Price (USD)** | **Total (USD)** | **Total (ZAR)** |
| --- | --- | --- | --- | --- | --- |
| **Compute Nodes** | Dell PowerEdge R760 (Intel Xeon Platinum 8468, 48C/96T) | 3 | $5,500 | $16,500 | R330,000 |
| **Memory** | 512GB DDR5 ECC (per node) | 3 | $2,000 | $6,000 | R120,000 |
| **Storage** | 2TB NVMe SSD (per node) | 3 | $250 | $750 | R15,000 |
| **Networking** | 100Gbps Ethernet | 3 | $600 | $1,800 | R36,000 |
| **Switch** | 100Gbps Ethernet Switch | 1 | $2,000 | $2,000 | R40,000 |
| **Total** |  |  |  | **$20,000** | **R400,000** |

🔹 **Justification:**

* **ICON needs high memory bandwidth**, so we chose **Intel Xeon Platinum 8468**, which supports **fast DDR5 RAM**.
* **3-node setup with 512GB RAM per node** ensures smooth large-scale weather simulations.
* **100Gbps networking** prevents bottlenecks in inter-node communication.

**HPC Cluster for SwiftSIM (Astrophysics Simulations)**

**🛠️ Hardware Selection:**

| **Component** | **Model** | **Qty** | **Unit Price (USD)** | **Total (USD)** | **Total (ZAR)** |
| --- | --- | --- | --- | --- | --- |
| **Compute Nodes** | Dell PowerEdge R760 (AMD EPYC 9334, 32C/64T) | 2 | $4,000 | $8,000 | R160,000 |
| **GPUs** | NVIDIA A40 48GB | 2 | $4,500 | $9,000 | R180,000 |
| **Memory** | 256GB DDR5 ECC (per node) | 2 | $1,200 | $2,400 | R48,000 |
| **Storage** | 1TB NVMe SSD (per node) | 2 | $250 | $500 | R10,000 |
| **Networking** | 25Gbps Ethernet | 2 | $600 | $1,200 | R24,000 |
| **Switch** | 25Gbps Ethernet Switch | 1 | $1,900 | $1,900 | R38,000 |
| **Total** |  |  |  | **$20,000** | **R400,000** |

🔹 **Justification:**

* **SwiftSIM is a hybrid CPU-GPU workload**, so we need **strong CPUs** + **high FP32/FP64 GPUs**.
* **NVIDIA A40 48GB** is **ideal for large-scale astrophysics models**.
* **25Gbps networking** is enough since SwiftSIM is more compute-heavy than network-dependent.

**HPC Cluster for MLPerf (AI & Deep Learning)**

**🛠️ Hardware Selection:**

| **Component** | **Model** | **Qty** | **Unit Price (USD)** | **Total (USD)** | **Total (ZAR)** |
| --- | --- | --- | --- | --- | --- |
| **Compute Nodes** | HPE ProLiant DL385 Gen11 (AMD EPYC 9334, 32C/64T) | 2 | $4,000 | $8,000 | R160,000 |
| **GPUs** | NVIDIA A100 80GB | 2 | $5,500 | $11,000 | R220,000 |
| **Memory** | 128GB DDR5 ECC (per node) | 2 | $600 | $1,200 | R24,000 |
| **Storage** | 2TB NVMe SSD (per node) | 2 | $250 | $500 | R10,000 |
| **Networking** | 100Gbps Ethernet | 2 | $800 | $1,600 | R32,000 |
| **Switch** | 100Gbps Ethernet Switch | 1 | $3,000 | $3,000 | R60,000 |
| **Total** |  |  |  | **$20,000** | **R400,000** |

🔹 **Justification:**

* **MLPerf needs maximum GPU throughput**, so we chose **NVIDIA A100 80GB (HPC-grade Tensor Cores)**.
* **AMD EPYC 9334** balances CPU performance for **preprocessing and data loading**.
* **100Gbps Ethernet ensures high-speed data transfer between nodes**.