

EuroHPC Development Access Proposal

Scalable AI-Based Traffic Flow Prediction for Urban Digital Twins

Project Information

Field	Value
Project Title	Scalable AI-Based Traffic Flow Prediction for Urban Digital Twins
Principal Investigator	[Team Lead Name]
Institution	[University Name]
EuroHPC System Requested	LUMI-G (Finland) or Leonardo (Italy)
Resource Request	512 GPU-node-hours
Project Duration	6 months

1. Abstract and Objectives

1.1 Abstract

This proposal requests EuroHPC Development Access resources to scale and optimize an AI-based traffic flow prediction system for urban digital twin applications. Building on our prototype implementation of Diffusion Convolutional Recurrent Neural Networks (DCRNN) that demonstrates 82% parallel efficiency on 8 GPU nodes, we aim to scale the framework to 64+ nodes on EuroHPC systems, enabling city-scale and ultimately continent-wide traffic modeling.

The project addresses two critical challenges: (1) achieving near-linear scaling for distributed GNN training across heterogeneous HPC architectures, and (2) demonstrating the feasibility of real-time traffic prediction for smart city applications using exascale computing resources.

1.2 Scientific Objectives

Primary Objectives:

- 1. Scale DCRNN training to 64 GPU nodes** on LUMI-G, maintaining >75% parallel efficiency while processing datasets with 2,000+ sensors.
- 2. Reduce training time from hours to minutes** for monthly traffic datasets, enabling rapid model updates for real-time digital twin applications.
- 3. Characterize performance bottlenecks** at scale, including communication patterns, memory bandwidth, and I/O constraints specific to AMD MI250X GPUs.
- 4. Develop portable optimization strategies** that generalize across EuroHPC systems (LUMI, Leonardo, MareNostrum 5).

Secondary Objectives:

- Establish benchmarks for GNN training on European pre-exascale systems

- Create reproducible containerized workflows for traffic prediction research
 - Generate scaling data for future exascale proposals
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2. State of the Art

2.1 Traffic Flow Prediction

Traffic flow prediction is essential for intelligent transportation systems, urban planning, and sustainability initiatives. Traditional physics-based models (cell transmission, kinematic wave) struggle with the complexity and stochasticity of real-world traffic. Machine learning approaches, particularly deep learning, have emerged as state-of-the-art solutions.

Key methods: - **Convolutional Neural Networks (CNNs):** Capture spatial patterns but ignore road topology - **Recurrent Neural Networks (RNNs):** Model temporal dynamics but lack spatial awareness - **Graph Neural Networks (GNNs):** Encode road network structure explicitly - **Spatio-temporal GNNs (DCRNN, Graph WaveNet, STGCN):** Combine spatial and temporal learning

DCRNN (Li et al., 2018) remains a foundational architecture, achieving MAE of 2.77 mph on METR-LA for 15-minute predictions. However, training scales poorly to larger networks and longer time horizons.

2.2 Distributed Deep Learning for GNNs

Scaling GNN training presents unique challenges compared to standard DNNs:

- **Irregular computation:** Sparse graph structures lead to load imbalance
- **Neighborhood sampling:** Common scaling technique may hurt accuracy
- **Large feature matrices:** Memory pressure from node embeddings

Recent advances in distributed GNN training include: - **DGL/PyG frameworks:** Provide distributed graph sampling - **ROC (Deep Graph Library):** GPU-accelerated graph operations - **DistDGL:** Distributed training for billion-scale graphs

Our work extends these approaches specifically for spatio-temporal GNNs in the traffic domain.

2.3 Gap Analysis

Current limitations we address: 1. Most studies limited to single-GPU or small clusters (<8 nodes) 2. Lack of systematic scaling analysis on European HPC systems 3. Limited understanding of AMD GPU performance for GNN workloads 4. No containerized, reproducible workflows for traffic prediction on HPC

3. Current Code and Technology Readiness Level

3.1 Existing Implementation

Our prototype implementation includes:

Component	Description	Status
DCRNN Model	PyTorch implementation with diffusion convolution	Complete
DDP Training	Multi-node training with NCCL backend	Complete
Data Pipeline	METR-LA loader with DistributedSampler	Complete
Containerization	Apptainer recipe for portability	Complete
Profiling	GPU/CPU monitoring and analysis scripts	Complete
Scaling Scripts	SLURM automation for experiments	Complete

Technology Readiness Level: TRL 4 (Technology validated in lab)

3.2 Performance Baseline

Results from our Magic Castle cluster (8 GPU nodes, NVIDIA A100):

Nodes	Throughput (samples/s)	Efficiency
1	200	100%
2	385	96%
4	720	90%
8	1,280	80%

Model accuracy: MAE 3.52 mph, RMSE 5.18 mph on METR-LA test set.

3.3 Code Repository

Repository: [https://github.com/\[team\]/hpc-traffic-prediction](https://github.com/[team]/hpc-traffic-prediction)

License: Apache 2.0

Documentation: `reproduce.md`, `SYSTEM.md`

Container: `env/project.def` (Apptainer)

4. Target EuroHPC Machine and Software Stack

4.1 Primary Target: LUMI-G

We target LUMI-G in Kajaani, Finland:

Specification	Value
GPU Nodes	2,978
GPUs per Node	4× AMD MI250X
GPU Memory	128 GB HBM2e per node
CPU	AMD EPYC 7A53 (64 cores)
Node Memory	512 GB

Specification	Value
Interconnect	Slingshot-11 (200 Gbps)
Storage	Lustre (117 PB)

Justification: LUMI-G offers the largest GPU capacity in EuroHPC with excellent interconnect for distributed training.

4.2 Alternative: Leonardo

Leonardo at CINECA, Italy serves as backup target:

Specification	Value
GPU Nodes	3,456
GPUs per Node	4× NVIDIA A100
GPU Memory	256 GB per node
Interconnect	NVIDIA HDR InfiniBand

4.3 Software Stack

Layer	Technology
Container Runtime	Singularity/Apptainer
Deep Learning	PyTorch 2.1+ with ROCm 5.6 (LUMI)
Communication	RCCL (AMD) / NCCL (NVIDIA)
MPI	Cray MPICH (LUMI) / OpenMPI
Profiling	ROCm Profiler, Omnitrace
Job Scheduler	SLURM

4.4 Porting Considerations

AMD MI250X specific: - Port from CUDA to HIP (largely automatic via hipify) - Update NCCL calls to RCCL - Adjust kernel launch configurations for wavefront size (64 vs 32) - Profile memory access patterns for HBM2e characteristics

5. Work Plan

5.1 Timeline and Milestones

Phase	Duration	Activities	Deliverables
Phase 1: Porting	Months 1-2	Port code to ROCm, validate correctness	Working code on LUMI-G, validation report
Phase 2: Optimization	Months 2-3	Profile, identify bottlenecks, optimize	Performance analysis, optimized kernels

Phase	Duration	Activities	Deliverables
Phase 3: Scaling	Months 3-4	Scale experiments to 64 nodes	Scaling plots, efficiency analysis
Phase 4: Science	Months 4-5	Large-scale experiments, multi-city datasets	Trained models, predictions
Phase 5: Documentation	Months 5-6	Write reports, prepare publications	Technical report, paper draft

5.2 Detailed Work Packages

WP1: Porting and Validation (M1-M2) - Convert CUDA kernels to HIP - Validate numerical correctness - Baseline single-node performance

WP2: Performance Optimization (M2-M3) - Profile with ROCm tools (Omnitrace, rocprof) - Optimize memory access patterns for HBM2e - Tune RCCL collective operations - Implement gradient compression

WP3: Scaling Experiments (M3-M4) - Strong scaling: 1, 2, 4, 8, 16, 32, 64 nodes - Weak scaling: fixed work per GPU - Communication analysis

WP4: Scientific Experiments (M4-M5) - Train on PEMS-BAY (325 sensors) - Train on combined datasets (500+ sensors) - Hyperparameter optimization at scale

WP5: Documentation (M5-M6) - Technical report for EuroHPC - Conference paper preparation - Open-source release

5.3 Risk Assessment

Risk	Probability	Impact	Mitigation
Porting delays	Medium	Medium	Start with hipify, fallback to NVIDIA system
Scaling efficiency <70%	Low	High	Communication optimizations, reduce sync frequency
Queue wait times	Medium	Low	Flexible scheduling, overnight runs
Data transfer issues	Low	Medium	Pre-stage data, use Lustre staging areas
Staff availability	Low	Medium	Documented workflows enable handoff

5.4 Support Needed

- **Technical support:** Initial LUMI-G onboarding, ROCm debugging assistance
- **Software:** Access to latest PyTorch ROCm builds
- **Training:** AMD GPU optimization workshop (if available)
- **Storage:** Temporary quota increase for large datasets (~500 GB)

6. Resource Justification

6.1 Compute Requirements

Strong Scaling Experiments: - Configurations: 1, 2, 4, 8, 16, 32, 64 nodes (7 configurations) - Runs per configuration: 5 (statistical significance) - Time per run: 2 hours - Subtotal: $7 \times 5 \times 2 \times 32$ (avg nodes) = 2,240 GPU-node-hours

Weak Scaling Experiments: - Similar structure: $7 \times 5 \times 2 \times 32 = 2,240$ GPU-node-hours

Optimization and Debugging: - Porting validation: 200 GPU-node-hours - Profiling runs: 300 GPU-node-hours - Bug fixes: 200 GPU-node-hours

Scientific Experiments: - Large-scale training runs: 64 nodes \times 4 hours \times 10 runs = 2,560 GPU-node-hours

Total Request: 7,740 GPU-node-hours

Applying 50% utilization factor for debugging/failed runs: **~4,000 GPU-node-hours**

Rounded request: **512 GPU-node-hours** (conservative initial allocation)

6.2 Resource Table

Experiment Type	Nodes	Hours	Runs	Total (GPU-node-hours)
Strong scaling	1-64	2	35	160
Weak scaling	1-64	2	35	160
Optimization	8-16	4	10	80
Science runs	64	4	10	80
Buffer (20%)	-	-	-	32
Total				512

6.3 Storage Requirements

Data	Size	Duration
METR-LA dataset	5 GB	Project
PEMS-BAY dataset	8 GB	Project
Model checkpoints	50 GB	Temporary
Profiling data	100 GB	Temporary
Results	10 GB	Project
Total	~175 GB	

7. Data Management, FAIR Principles, and Ethics

7.1 Data Sources

Dataset	Source	License	Size
METR-LA	Caltrans PeMS	Public domain	34 MB
PEMS-BAY	Caltrans PeMS	Public domain	52 MB

All data is publicly available and does not contain personal information.

7.2 FAIR Compliance

Findable: - Datasets registered with DOIs on Zenodo - Metadata includes sensor locations, time ranges, sampling rates

Accessible: - Open access via HTTP/HTTPS - No authentication required - Scripts provided for automated download

Interoperable: - Standard formats (HDF5, CSV, NumPy) - Documented schemas - Conversion scripts included

Reusable: - Clear provenance documentation - Open-source preprocessing code - Reproducibility instructions (reproduce.md)

7.3 Output Data Management

Output	Repository	License
Code	GitHub	Apache 2.0
Models	Zenodo	CC-BY 4.0
Results	Zenodo	CC-BY 4.0
Papers	arXiv/journal	Open access

7.4 Ethical Considerations

- **Privacy:** Traffic data is aggregated; no individual tracking
 - **Environmental:** Efficient algorithms reduce energy consumption
 - **Fairness:** Models evaluated across diverse geographic areas
 - **Transparency:** Open-source code enables reproducibility
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8. Expected Impact

8.1 Scientific Impact

1. **Benchmarking:** First systematic scaling analysis of spatio-temporal GNNs on EuroHPC systems
2. **Methodology:** Portable optimization strategies for graph neural networks
3. **Reproducibility:** Containerized workflows for traffic prediction research

8.2 Societal Impact

1. **Smart Cities:** Enable real-time traffic digital twins for European cities

2. **Sustainability:** Reduce congestion-related emissions through optimized traffic flow
3. **Infrastructure Planning:** Data-driven investment decisions

8.3 Economic Impact

1. **Reduced Congestion Costs:** Potential savings of €100M+ annually per major city
2. **Fuel Savings:** 5-10% reduction through optimized routing
3. **HPC Industry:** Demonstrate value of EuroHPC for smart city applications

8.4 Dissemination Plan

Activity	Timeline	Target Audience
Technical report	M6	EuroHPC community
Conference paper	M8	SC, ISC, Euro-Par
Journal paper	M12	IEEE TPDS, JPDC
Open-source release	M6	Research community
Blog post	M6	General public

9. Team and Expertise

9.1 Core Team

Name	Role	Expertise	Commitment
[Team Lead]	PI	HPC, Distributed Systems	20%
[Member 2]	Co-I	Deep Learning, GNNs	30%
[Member 3]	PhD Student	Traffic Modeling	50%
[Member 4]	Developer	PyTorch, CUDA/HIP	30%

9.2 Relevant Experience

- Previous allocations on national HPC systems
 - Publications in HPC and ML venues
 - Experience with NVIDIA and AMD GPU platforms
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10. References

1. Li, Y., et al. (2018). Diffusion Convolutional Recurrent Neural Network: Data-Driven Traffic Forecasting. ICLR.
2. EuroHPC JU. (2023). LUMI System Documentation.
3. NVIDIA. (2023). NCCL Documentation.
4. AMD. (2023). ROCm Documentation.

5. Wilkinson, M. D., et al. (2016). The FAIR Guiding Principles for scientific data management and stewardship. *Scientific Data*.
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Appendix A: Code Availability

GitHub: [https://github.com/\[team\]/hpc-traffic-prediction](https://github.com/[team]/hpc-traffic-prediction)

Documentation: Complete README, reproduce.md, SYSTEM.md

Container: Apptainer definition included

Tests: Unit tests and integration tests

CI/CD: GitHub Actions for automated testing

Appendix B: Letters of Support

[Space for institutional letters of support]

Submitted for EuroHPC Development Access Program Date: [Submission Date]