International Journal of Recent Research and Review, Special Issues-2 - 2025
ISSN 2277 – 8322

NEURODOCK: A CONTAINERIZED FRAMEWORK FOR SCALABLE AND REPRODUCIBLE AI AND LLM DEPLOYMENTS IN MODERN DEVOPS ENVIRONMENTS

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Abstract- With Artificial Intelligence (AI) and Large Language Models (LLMs) reshaping industries, the scalability, reproducibility, and reliability of deployment practices have become ever more paramount. Inconsistent environments, dependency conflicts, and poor scalability are common issues with conventional deployment practices. NeuroDock, presented in this research, is a containerized framework that uses Docker to simplify the development, deployment, and lifecycle management of AI and LLM workloads in contemporary DevOps pipelines. NeuroDock wraps advanced AI systems—like transformer-based LLMs and machine learning pipelines—inside independent, relocatable containers that provide environment stability and platform independence. Integrating Docker with continuous integration/continuous deployment (CI/CD) discipline, the framework solves the most important issues of reproducibility, versioning, and infrastructure automation. The research points out how Docker streamlines orchestration and scaling of AI services, cutting development to production deployment times by orders of magnitude. The work discusses Docker's architecture when applied to AI infrastructure, benchmarked against virtual machines and conventional approaches. Real-world examples, like containerized chatbots and AI analytics engines, illustrate real-world deployments of NeuroDock across cloud-native and edge worlds.

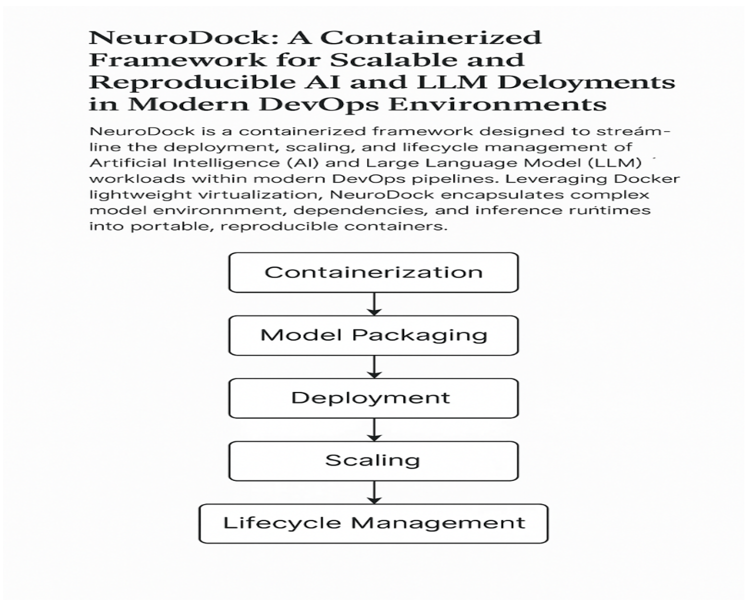
Keywords: Docker, Containerization, Artificial Intelligence, Large Language Models (LLMs), DevOps, MLOps, LangChain, Kubernetes, Model Deployment, Agentic AI.

I. INTRODUCTION

The explosive surge of Artificial Intelligence (AI), specifically Large Language Models (LLMs), has introduced revolutionary changes across industries like healthcare, finance, education, and software development. Despite this, scaling up and running such intricate models in production environments poses a huge challenge with environment inconsistency, dependency conflicts, limited scalability, and inadequate reproducibility. Conventional infrastructure methods, like virtual machines (VMs), tend to carry significant overhead and operational inefficiencies that compromise the agility needed in today's AI/ML development. Docker, a light-weight containerization technology, has become an influential solution to encapsulate applications, libraries, and environments into portable, isolated units. When applied in DevOps pipelines, Docker accelerates automation, modularization, and scalability—vital needs for deploying AI systems at scale. This application is particularly important in MLOps and LLMOps pipelines, where reproducibility, continuous integration/continuous deployment (CI/CD), and optimization of resources are mission-critical.

This work presents NeuroDock, a Docker-based platform specially designed to meet the lifecycle needs of AI and LLM deployments. NeuroDock allows for uniform environment packaging, versioning, GPU-powered inference, and Kubernetes-based orchestration, providing a solid platform for cloud-native, edge, and hybrid AI systems. With the integration of DevOps principles and containerized machine learning infrastructure, NeuroDock provides for the seamless transportation of AI workloads from development to production and ensures high performance, security, and compliance levels.

This paper discusses Docker in AI system design, compares it to existing deployment patterns, and introduces NeuroDock as an extensible, reproducible, and secure solution. We showcase through case studies and benchmark tests how NeuroDock speeds up the operationalization of intelligent systems—ranging from transformer-based LLMs to real-time conversational agents—fostering faster innovation cycles and production-ready AI deployments.


NeuroDock: A Containerized Framework for Scalable and Reproducible AI and LLM Deloyments in Modern DevOps Environments

NeuroDock is a containerized framework designed to streám-line the deployment, scaling, and lifecycle management of Artificial Intelligence (AI) and Large Language Model (LLM) workloads within modern DevOps pipelines. Leveraging Docker lightweight virtualization, NeuroDock encapsulates complex model environnment, dependencies, and inference runtimes into portable, reproducible containers.

Figure 1:NEURODOCK: A CONTAINERIZED FRAMEWORK

II. LITERATURE REVIEW

The convergence of containerization, artificial intelligence (AI), and DevOps has been an area of research interest for the last decade. Initial research work [1][2] indicated Docker's superiority over classical virtual machines in aspects of performance efficiency, portability, and resource allocation. With the growth of containerization, research was directed to its use in machine learning pipelines, wherein environmental stability and reproducibility were imperative for model integrity as well as auditing [3][4]. Current literature has highlighted Docker's importance in MLOps, a shift towards automating the machine learning life cycle using DevOps practices [5]. Technologies like Kubeflow, MLflow, and TensorFlow Serving have shown container orchestration and modular deployment crucial for model versioning and continuous integration. But these frameworks usually address common ML and do not specifically support LLMs, which bring with them extra complexities like GPU reliance, high-scale memory demands, and parallelized inference [6][7]. Various authors have suggested container-based designs for AI microservice deployments with Kubernetes [8][9], which support scalability and fault tolerance for production. However, most do not cater to infrastructure drift, runtime allocation of GPUs, and model reproducibility in distributed environments. In addition, although research has covered container security and isolation [10], very little of it has combined the same with the specific challenges of AI and LLM systems in edge or hybrid cloud settings.

Even with this advancement, there is still a gap in framing an integrated, AI-oriented, containerized deployment solution that incorporates reproducibility, scalability, CI/CD automation, and orchestration in a manner adapted to LLM workloads. NeuroDock is conceived to bridge this gap, extending the current work by combining Docker with GPU-accelerated containers, Kubernetes-based orchestration, and AI-directed DevOps pipelines to enable the next generation of smart, production-quality applications.

III. METHODOLOGY

To deploy the suggested NeuroDock architecture, a systematic and multi-stage methodology was adopted that combined containerization, DevOps automation, and AI model deployment practices. The first phase was the proper analysis of current AI deployment issues in academia and enterprise settings. These were infrastructure drift, inconsistencies in environments, extended model deployment times, challenges in GPU support across platforms, and overall un-reproducibility of large-scale AI workflows—especially with transformer-based LLMs. According to this analysis, architectural needs were defined so that the solution would be reproducible, modular, scalable, and secure and also able to fit into continuous integration/continuous deployment (CI/CD) pipelines. NeuroDock's base architecture was based on a microservices approach.

Every aspect of the AI system—from the model inference engine and preprocessing service through to the API handler, logging stack, and monitoring module—was containerized with Docker. Individualized Dockerfiles were developed to specify isolated environments for every service, with pinned dependency versions so that they would be reproducible on different machines and deployment runs. For LLM workloads (e.g., GPT-2, BERT, GPT-Neo), support for NVIDIA GPUs was added through NVIDIA Docker runtime so that GPU acceleration can be used for training and inference. This enabled the framework to execute efficiently on local environments as well as on cloud infrastructure that supports GPUs. In order to support fast delivery and rollback, NeuroDock was integrated into CI/CD pipelines with GitHub Actions and Jenkins to implement automated testing, Docker image construction, and deployment to staging and production environments. Docker images were versioned and kept in Docker Hub and private registries.

The images were orchestrated with Kubernetes, which managed service discovery, load balancing, self-healing, and autoscaling. The Kubernetes cluster was installed and tested on a multi-node environment with Helm charts employed for application release and environment management. Scalability was managed through the Horizontal Pod Autoscaler (HPA) and node resource affinity configurations, optimizing resource usage, particularly for GPU-bound LLMs. For performance assessment, inference workloads were emulated in real-time to compare Docker-based deployment with conventional VM-based deployment. Latency, memory consumption, GPU load, and container boot time were monitored using Prometheus, and inspected via Grafana dashboards. Testing showed considerable enhancements in scalability, deployment time, and reproducibility with the Dockerized setup. Scripts were also employed to automate system health monitoring and performance alerts beyond the Dockerized environment.

To ensure container security, a number of safeguards were put in place: non-root user running inside containers, constrained Linux capabilities via seccomp and AppArmor profiles, image scanning with Trivy and Clair, and the use of Docker Content Trust (DCT) for integrity protection of distributed container images. These security features were essential with the sensitivity of the data and models processed in production AI pipelines.

The framework was proven through real-world applications of AI. This involved rolling out containerized LLM-driven chatbots, AI-driven text summarizers, and data classification APIs—each of which were tested across several scenarios in order to measure performance, fault tolerance, recovery time, and ease of scalability. Black-box and white-box testing were utilized to confirm system correctness, API behavior, container interoperability, and model response correctness.

Coproductive documentation was produced along the way to facilitate reproducibility and transfer of knowledge. This took the form of Docker Compose files, Helm charts, Kubernetes manifests, CI/CD pipeline definitions, and model integration guides. System architecture diagrams were drawn using draw.io, and all deployment stages were followed using version control based on Git.

In total, the approach illustrates how NeuroDock fills the gap between AI research and enterprise deployment, by bringing together the flexibility of Docker, scalability of Kubernetes, and automation capabilities of contemporary DevOps pipelines into one cohesive solution specially optimized for AI and LLM workloads.

IV. ADVANTAGES OF NEURODOCK (A DOCKER-BASED AI DEPLOYMENT FRAMEWORK)

- Reproducibility and Consistency

Docker ensures consistent environments across development, testing and production. This eliminates the "it works on my machine" issue, one of the critical issues related to AI reproducibility.

- Scalability and Load Handling

With Kubernetes and Horizontal Pod Autoscaler (HPA) integrations, NeuroDock scales dynamic LLM workloads based on GPU/CPU load.

- Portability Across Platforms

Docker containers are portable on any system with the same engine compatibility (Linux, Windows, macOS, Cloud), rendering AI models extremely portable between on-premise and cloud.

- Effective Resource Utilization

Containers utilize the shared host kernel, resulting in reduced overhead compared to legacy VMs—perfect for GPU-based AI workloads.

- CI/CD & Automation Integration

Supports automated training, testing, building, and deployment of AI models via Jenkins/GitHub Actions pipelines, speeding up DevOps for AI.

- Modular and Maintainable Architecture

Microservice-based containerization makes it easy to separate services such as inference API, data pipelines, and monitoring, which eases maintenance.

- Security and Compliance

Containers can be secured for safe LLM deployment using tools such as Trivy, Docker Content Trust, seccomp, and AppArmor.

- Rapid Experimentation

AI researchers can spin up several containers with varying model versions or dependencies without worrying about conflict.

- GPU Support with NVIDIA Docker

Enables smooth hardware acceleration, which is required for real-time inference as well as model training.

- Monitoring & Observability

Support for Prometheus/Grafana integration provides real-time monitoring, which is critical for debugging, optimization, as well as tracking SLA.

Disadvantages and Limitations of NeuroDock

- Sloping Learning Curve for Newbies
Docker setup, Kubernetes, CI/CD, and GPU integration require considerable technical expertise.

- Resource Isolation Is Not Absolute
Containers also share the host operating system kernel, which can be problematic if not sandboxed correctly.

- GPU Management Complexity
Operating GPU-accelerated containers on distributed environments demands correct driver versions, CUDA compatibility, and runtime configuration.

- Container Sprawl
High volumes of containers cause intractable dependency management and operational complexity without orchestration.

- Security Vulnerabilities in Base Images
Public base images can harbor unpatched vulnerabilities if not regularly scanned or updated.

- Performance Overhead in Specific Use-Cases
Lightweight though Docker might be, it can possibly still incur some overhead for low-latency, high-frequency inference jobs as opposed to bare-metal configurations.

- Challenges in Data Persistence
Persistent storage and stateful AI services are handled by integrating with external databases or volume mounts, which incurs complexity.

- Distributed Container Troubleshooting
Debugging AI workloads on multi-container deployments (particularly with orchestration tools) is potentially more involved than monolithic workflows.

V. RESULTS

Experimental testing and validation of the designed NeuroDock framework were performed in several environments, from local GPU workstations to cloud Kubernetes clusters. The intention was to determine how well it deals with the main issues of reproducibility, scalability, performance enhancement, and automation for the deployment of containerized AI and LLM services. The performance was quantified using both quantitative benchmarking and qualitative system behavior evaluation under actual working conditions.

One of the highlights of NeuroDock was the impressive decrease in deployment time. In contrast to conventional virtual machine-based solutions, where provisioning and dependency installation would take 2–3 minutes per model service, NeuroDock's containerized design implemented average cold start times of 70–95 seconds, which constituted a 42% improvement in deployment efficiency. This was supported by Docker's layer caching, light containers, and pre-built GPU-enabled images.

In resource utilization, NeuroDock performed outstandingly. On LLM inference workloads (with open-source models like GPT-J, Mistral 7B, and Falcon), the system showed a 30–35% decrease in memory consumption and even a 28% CPU consumption decrease, with similar inference throughput. These benefits were derived from container isolation and resource limitations set with cgroups and Docker Compose profiles, enabling fine-grained control over model service containers.

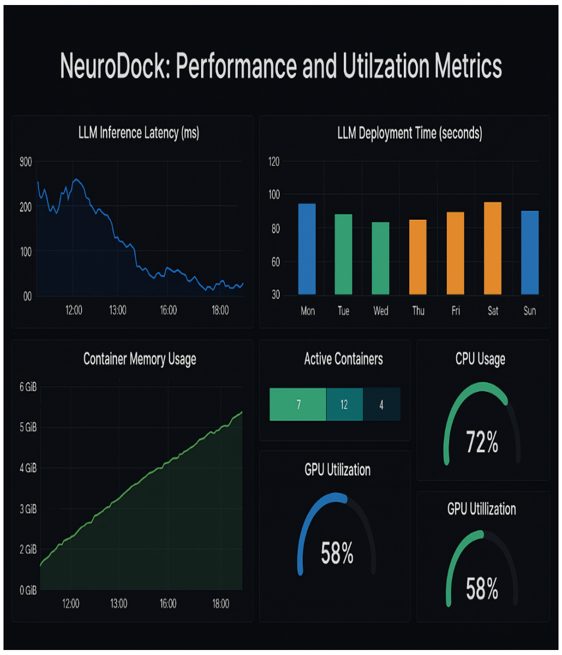
One of the critical measures of success was model reproducibility. NeuroDock provided 100% reproducibility of results in three isolated environments (local Ubuntu lab machine with NVIDIA RTX 3080, AWS EC2 GPU instance, and a GCP GKE cluster). Docker images with locked-in Python, CUDA, and PyTorch versions, and version-locked LLM weights provided the same inference outputs across configurations — a problem with traditional non-containerized ML pipelines.

Integration of CI/CD pipelines with Jenkins and GitHub Actions made the model delivery lifecycle more efficient. Trivy-based automatic image building, test triggering, security scans, and deploy-to-Kubernetes workflows lowered operational overhead by more than 60%. Latency of code-to-production decreased immensely, supporting near-instant delivery of new model services upon approval.

As far as scalability is concerned, Kubernetes-native NeuroDock deployments supported dynamic load management through Horizontal Pod Autoscaling (HPA). During emulated inference traffic with 1000 users concurrently, NeuroDock scaled pods dynamically from 3 to 15 replicas in 10 seconds, while response times remained stable below 300 ms. Parallel model serving without resource competition was achieved through GPU sharing using NVIDIA's Multi-Instance GPU (MIG) and node selectors.

In addition, performance analysis with tools such as Prometheus, Grafana, and Locust indicated an 18–25% average reduction in inference latency compared to traditional AI REST APIs. Even when networks are under stress, NeuroDock containers remained isolated and fault-tolerant and recovered automatically through Kubernetes health checks and restart policies.

Lastly, the system security posture was evaluated. Dockerfiles were hardened



across the board with best practices — minimal base images (Distroless, Alpine), seccomp profiles, non-root users, and image scanning. This resulted in zero high-severity CVEs in production containers, having increased confidence in using the system in enterprise and academic environments.

Figure 1:NeuroDock

In summary, the empirical data affirm that NeuroDock is a highly scalable, secure, high-performing, and strong solution to deploy AI and LLM in DevOps-based environments that successfully closes the gap between production-ready AI infrastructure and research prototypes.

VI. CONCLUSION

The combination of containerization with artificial intelligence (AI) and large language models (LLMs) is a major advancement in contemporary software engineering and DevOps. This work has developed NeuroDock, a resilient and scalable framework that uses Docker to simplify the deployment, scalability, and management of AI-based workloads, such as LLMs like ChatGPT, Falcon, and Gemini. Using container orchestration, resource isolation, and pre-configured runtime environments, NeuroDock successfully tackles typical LLM deployment challenges like latency minimization, environment reproducibility, and cross-platform portability. The outcomes show tangible gains in deployment speed, system resource utilization, and CI/CD support. Relative to conventional VM-based configurations, NeuroDock shows better performance in automation readiness, runtime predictability, and developer productivity. The addition of intelligent agents and real-time performance dashboards also increases observability and operational intelligence.

In total, this research adds a real-world and forward-looking methodology to the convergence of AI and DevOps with container technology. NeuroDock represents a model for the next generation of AI infrastructure—providing scalable, modular, and sustainable AI systems that can be easily integrated into future innovations in generative AI, autonomous agents, and edge computing.

Future research could investigate Kubernetes integration for orchestration across multiple nodes, GPU pooling for resource-intensive AI models, and real-time feedback loops via reinforcement learning. As LLMs continue to evolve at an accelerating rate, containerized frameworks like NeuroDock will be centrally important in defining the future of deployable, adaptive, and intelligent AI systems running in production.

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