Multi-Agent NWB Conversion Pipeline - Technical Specification

Executive Summary

This document provides complete technical specifications for implementing a multi-agent system for converting heterogeneous neuroscience data into the Neurodata Without Borders (NWB) format using the Model Context Protocol (MCP) as the core communication framework.

1. System Architecture Overview

1.1 Core Technology Stack

- Agent Framework: MCP (Model Context Protocol) for inter-agent communication
- Runtime Environment: Python 3.10+
- Orchestration: Apache Airflow or Prefect for workflow management
- Message Queue: RabbitMQ or Redis for async communication
- Data Storage: MinIO for object storage, PostgreSQL for metadata
- Containerization: Docker & Kubernetes for deployment

1.2 MCP Implementation Strategy

```
python
# MCP Server Configuration Structure
{
    "protocol_version": "1.0",
    "server_info": {
        "name": "nwb-conversion-pipeline",
        "version": "0.1.0",
        "capabilities": {
            "tools": true,
            "resources": true,
            "prompts": true
        }
    },
    "agents": [
        "conversation_agent",
        "evaluation_agent",
        "tuie_agent"
    ]
}
```

2. Agent Specifications

2.1 Conversation Agent

Purpose

Entry point for user interaction, metadata collection, and requirement gathering.

MCP Implementation

```
python
class ConversationAgentMCP:
  def __init__(self):
    self.mcp_server = MCPServer(
       name="conversation_agent",
       version="1.0.0"
    self.tools = [
       "gather_dataset_info",
       "extract_metadata",
       "validate_user_input",
       "query_knowledge_graph"
  async def handle_request(self, request: MCPRequest):
     # Request structure
       "method": "conversation/initiate",
       "params": {
         "user_id": str,
         "dataset_path": str,
         "metadata": dict,
         "missing_fields": list
```

API Endpoints

- (POST /conversation/start) Initialize conversation session
- (POST /conversation/metadata) Submit metadata
- (GET /conversation/status/{session_id}) Get conversation status
- POST /conversation/validate Validate collected information

Data Structures

```
python
@dataclass
class ConversationSession:
  session_id: str
  user_id: str
  timestamp: datetime
  dataset_info: DatasetInfo
  metadata_status: MetadataStatus
  missing_fields: List[str]
  ai_suggestions: List[Suggestion]
@dataclass
class DatasetInfo:
  path: str
  format: str
  size_bytes: int
  file_count: int
  data_types: List[str]
  sampling_rate: Optional[float]
  channels: Optional[int]
```

Integration Points

- Knowledge Graph: Query for existing metadata patterns
- **LinkML Schema**: Validate metadata against schemas
- **User Interface**: WebSocket for real-time interaction

2.2 Generation Agent (Conversion Agent)

Purpose

Execute the actual data conversion using NeuroConv, manage transformation pipeline.

MCP Implementation

-		
python		

```
class GenerationAgentMCP:
  def __init__(self):
    self.mcp_server = MCPServer(
       name="generation_agent",
       version="1.0.0"
    self.neuroconv = NeuroConvInterface()
  async def convert_dataset(self, request: MCPRequest):
     # Request structure
       "method": "conversion/execute",
       "params": {
         "session_id": str,
         "input_path": str,
         "output_path": str,
         "conversion_config": dict,
         "metadata": dict,
         "provenance": dict
     # Response structure
       "status": "success|processing|failed",
       "nwb_file_path": str,
       "conversion_log": str,
       "warnings": list,
       "provenance_record": dict
```

Conversion Pipeline Steps

1. Data Interface Selection

```
python

def select_data_interface(data_format: str) -> DataInterface:
    interfaces = {
        "blackrock": BlackrockInterface,
        "intan": IntanInterface,
        "openephys": OpenEphysInterface,
        "spikeglx": SpikeGLXInterface
    }
    return interfaces.get(data_format)
```

2. Metadata Injection

```
python
def inject_metadata(nwbfile: NWBFile, metadata: dict):
  # Add subject information
  # Add experiment metadata
  # Add device information
  # Add electrode configuration
  # Mark AI-suggested fields
```

3. Provenance Tracking

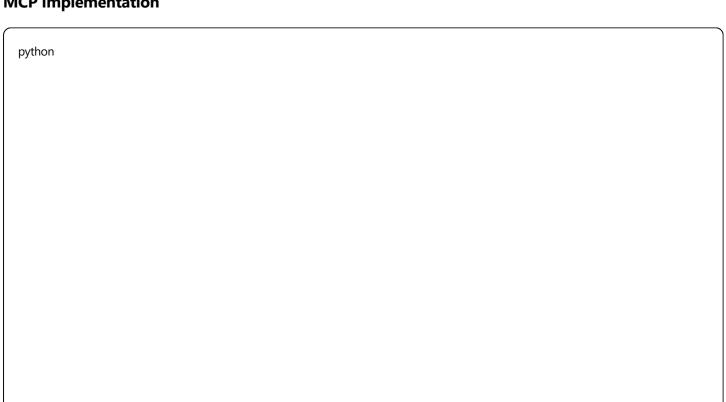
```
python
@dataclass
class ProvenanceRecord:
  conversion_id: str
  timestamp: datetime
  source_files: List[str]
  conversion_parameters: dict
  tool_versions: dict
  user_modifications: List[Modification]
  ai_suggestions_applied: List[str]
```

2.3 Evaluation Agent

Purpose

Validate generated NWB files for compliance and quality.

MCP Implementation



```
class EvaluationAgentMCP:
    def __init__(self):
        self.mcp_server = MCPServer(
            name="evaluation_agent",
            version="1.0.0"
    )
        self.inspector = NWBInspector()

async def validate_nwb(self, request: MCPRequest):
    # Request structure
    {
        "method": "validation/execute",
        "params": {
            "nwb_file_path": str,
            "validation_level": "basic|comprehensive|custom",
            "custom_checks": list
        }
    }
}
```

Validation Checks

```
python
class ValidationSuite:
  def __init__(self):
     self.checks = [
       SchemaComplianceCheck(),
       BestPracticesCheck(),
       MetadataCompletenessCheck(),
       DataIntegrityCheck(),
       TimeSeriesValidation(),
       UnitConsistencyCheck()
  async def run_validation(self, nwb_file: str) -> ValidationReport:
     results = []
     for check in self.checks:
       result = await check.validate(nwb_file)
       results.append(result)
     return ValidationReport(results)
```

Error Classification

```
class ErrorSeverity(Enum):

CRITICAL = "critical" # Must fix before proceeding

WARNING = "warning" # Should fix but not blocking

INFO = "info" # Suggestions for improvement

@dataclass

class ValidationError:
    severity: ErrorSeverity
    location: str
    message: str
    suggested_fix: Optional[str]
    auto_fixable: bool
```

2.4 Tool Use Instance Evaluator (TUIE)

Purpose

Meta-validator ensuring correct and efficient tool usage across the pipeline.

MCP Implementation

```
python

class TUIEAgentMCP:

def __init__(self):
    self.mcp_server = MCPServer(
        name="tuie_agent",
        version="1.0.0"
    )
    self.performance_metrics = {}

async def evaluate_tool_usage(self, request: MCPRequest):
    # Monitor tool invocations
    # Analyze performance metrics
    # Suggest optimizations
    # Detect redundant operations
```

Monitoring Metrics

python			

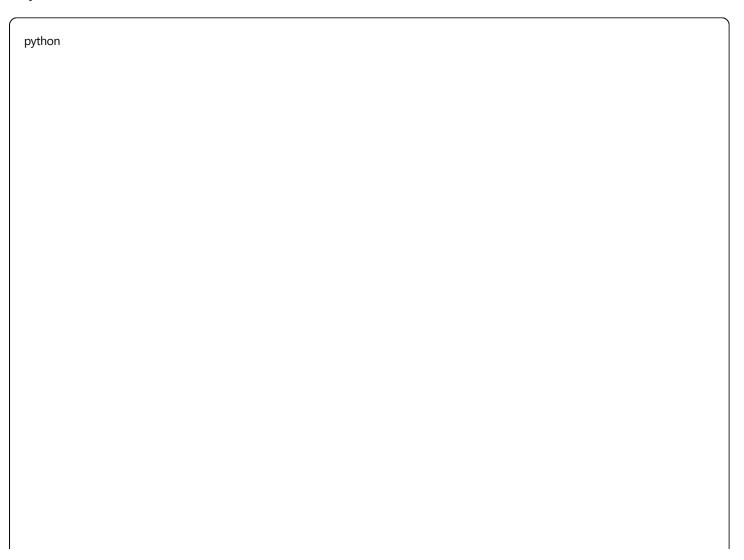
@dataclass
class ToolUsageMetrics:
 tool_name: str
 invocation_count: int
 average_duration: float
 error_rate: float
 resource_usage: ResourceMetrics
 optimization_suggestions: List[str]

@dataclass
class ResourceMetrics:
 cpu_usage: float
 memory_usage: float
 disk_io: float
 network_io: float

3. Intermediate Processes Specifications

3.1 Data Preprocessing and Analysis

Implementation



```
class DataPreprocessor:
  def __init__(self):
    self.supported_formats = [
       'dat', 'bin', 'continuous', 'nsx', 'nev',
       'rhd', 'rhs', 'oebin', 'kwik'
  async def preprocess(self, input_data: InputData) -> ProcessedData:
     # 1. Format detection
    format_type = self.detect_format(input_data)
     # 2. Data validation
    validation_result = self.validate_data_integrity(input_data)
     # 3. Standardization
    standardized = self.standardize_format(input_data, format_type)
     # 4. Quality checks
     quality_report = self.run_quality_checks(standardized)
    return ProcessedData(
       data=standardized.
       format=format_type,
       quality_report=quality_report
```

Data Standardization Pipeline

```
python

class StandardizationPipeline:
    stages = [
        SamplingRateNormalization(),
        ChannelReordering(),
        UnitConversion(),
        TimeAlignement(),
        FilteringOptional(),
        ArtifactDetection()
    ]

async def process(self, data: np.ndarray) -> np.ndarray:
    for stage in self.stages:
        data = await stage.process(data)
        return data
```

3.2 Metadata Extraction

Knowledge Graph Integration

```
python
class MetadataExtractor:
  def __init__(self):
    self.kg_client = KnowledgeGraphClient(
       endpoint="http://kg-service:8080",
       auth=KGAuth()
    self.linkml_validator = LinkMLValidator()
  async def extract_and_enrich(self, raw_metadata: dict) -> EnrichedMetadata:
     # 1. Extract from file headers
    file_metadata = self.extract_from_headers()
     # 2. Query knowledge graph
     kg_suggestions = await self.kg_client.query_similar(file_metadata)
     # 3. Apply LinkML schema
    validated = self.linkml_validator.validate(file_metadata)
     # 4. Mark provenance
    return EnrichedMetadata(
       user_provided=raw_metadata,
       extracted=file_metadata,
       ai_suggested=kg_suggestions,
       provenance=self.create_provenance()
```

LinkML Schema Definition

yaml			

```
# nwb_metadata_schema.yaml
id: https://example.org/nwb-metadata
name: nwb-metadata-schema
prefixes:
 nwb: https://www.nwb.org/
classes:
 Subject:
  attributes:
   subject_id:
    required: true
    range: string
   species:
    required: true
    range: Species
   age:
    range: string
    pattern: "^P\d+[YMD]$" # ISO 8601 duration
    range: Sex
 Device:
  attributes:
   name:
    required: true
   manufacturer:
    range: string
   model:
    range: string
```

3.3 Data Content Analysis

Signal Classification

python Python

3.4 Output and Reporting

Report Generation

```
class ReportGenerator:
    def __init__(self):
        self.template_engine = Jinja2Engine()

async def generate_reports(self, conversion_result: ConversionResult):
    reports = {
        'quality_report': self.generate_quality_report(conversion_result),
        'provenance_log': self.generate_provenance_log(conversion_result),
        'validation_report': self.generate_validation_report(conversion_result),
        'user_summary': self.generate_user_summary(conversion_result)
}

return reports
```

Quality Report Structure

json

```
"report_id": "uuid",
"timestamp": "2024-01-01T00:00:00Z",
"dataset_info": {
  "original_format": "string",
  "file_count": 0,
  "total_size_mb": 0.0
"conversion_metrics": {
  "duration_seconds": 0.0,
  "data_integrity": "preserved|modified|degraded",
  "metadata_completeness": 0.95
"validation_results": {
  "schema_compliance": true,
  "best_practices_score": 0.85,
  "warnings": [],
  "errors": []
},
"provenance": {
  "tool_versions": {},
  "user_modifications": [],
  "ai_suggestions_applied": []
```

3.5 Evaluation and Refinement

Feedback Loop Implementation

```
python
```

```
class RefinementLoop:
  def __init__(self):
    self.max iterations = 5
    self.improvement_threshold = 0.1
  async def refine(self, nwb_file: NWBFile, errors: List[ValidationError]):
    iteration = 0
    current_score = self.calculate_quality_score(nwb_file)
    while iteration < self.max_iterations:
       # Attempt automatic fixes
       auto_fixed = await self.apply_auto_fixes(nwb_file, errors)
       # Request human input for critical errors
       if self.has_critical_errors(errors):
         human_fixes = await self.request_human_input(errors)
         nwb_file = self.apply_human_fixes(nwb_file, human_fixes)
       # Re-validate
       new_errors = await self.validate(nwb_file)
       new_score = self.calculate_quality_score(nwb_file)
       # Check improvement
       if new_score - current_score < self.improvement_threshold:</pre>
         break
       errors = new_errors
       current_score = new_score
       iteration += 1
    return nwb_file, errors
```

4. Tools and Libraries Integration

4.1 NeuroConv Tool Integration

Configuration

```
class NeuroConvIntegration:
  def __init__(self):
     self.config = {
       "version": "0.4.0",
       "interfaces": {
          "blackrock": {
            "enabled": true,
            "options": {}
          },
          "intan": {
            "enabled": true,
            "options": {}
       },
       "conversion_options": {
          "stub_test": false,
          "verbose": true,
          "compression": "gzip",
          "compression_opts": 4
```

Custom DataInterface Implementation

```
python

class CustomDataInterface(BaseDataInterface):
    def __init__(self, file_path: str, **kwargs):
        super().__init__(file_path=file_path, **kwargs)

def get_metadata(self) -> dict:
    # Extract metadata specific to custom format
    pass

def get_metadata_schema(self) -> dict:
    # Return LinkML schema for validation
    pass

def run_conversion(self, nwbfile: NWBFile, metadata: dict):
    # Implement conversion logic
    pass
```

4.2 Knowledge Graph Integration

Graph Database Schema

```
// Neo4j schema for neuroscience metadata

CREATE CONSTRAINT subject_id ON (s:Subject) ASSERT s.id IS UNIQUE;

CREATE CONSTRAINT device_name ON (d:Device) ASSERT d.name IS UNIQUE;

CREATE CONSTRAINT experiment_id ON (e:Experiment) ASSERT e.id IS UNIQUE;

// Relationships

(s:Subject)-[:PARTICIPATED_IN]->(e:Experiment)

(e:Experiment)-[:USED_DEVICE]->(d:Device)

(e:Experiment)-[:HAS_RECORDING]->(r:Recording)

(r:Recording)-[:HAS_METADATA]-> (m:Metadata)
```

Query Interface

```
python
class KnowledgeGraphQuery:
  def __init__(self):
    self.driver = GraphDatabase.driver(
       "bolt://localhost:7687",
       auth=("neo4j", "password")
  async def find_similar_experiments(self, metadata: dict) -> List[dict]:
    query = """
    MATCH (e:Experiment)-[:HAS_METADATA]->(m:Metadata)
    WHERE m.species = $species
    AND m.recording_type = $recording_type
    RETURN e, m
    LIMIT 10
    with self.driver.session() as session:
       result = session.run(query, metadata)
       return [record.data() for record in result]
```

4.3 NWB Inspector Integration

Custom Validation Rules

```
class CustomValidationRules:
  def __init__(self):
    self.rules = [
         "name": "electrode_table_completeness",
         "severity": "warning",
         "check": self.check_electrode_table
       },
         "name": "timeseries_sampling_rate",
         "severity": "error",
         "check": self.check_sampling_rates
  def check_electrode_table(self, nwbfile: NWBFile) -> ValidationResult:
     # Check if all required electrode properties are present
    pass
  def check_sampling_rates(self, nwbfile: NWBFile) -> ValidationResult:
     # Verify sampling rates are consistent
    pass
```

5. MCP Communication Protocol

5.1 Message Format

```
ijson

{
    "jsonrpc": "2.0",
    "id": "unique-request-id",
    "method": "agent/action",
    "params": {
        "session_id": "session-uuid",
        "data": {},
        "metadata": {},
        "options": {}
    }
}
```

5.2 Inter-Agent Communication Flow

```
class MCPOrchestrator:
  def __init__(self):
    self.agents = {
       "conversation": ConversationAgentMCP(),
       "generation": GenerationAgentMCP(),
       "evaluation": EvaluationAgentMCP(),
       "tuie": TUIEAgentMCP()
    self.message_bus = MessageBus()
  async def process_conversion(self, request: ConversionRequest):
     # 1. Conversation phase
    metadata = await self.agents["conversation"].gather_metadata(request)
    # 2. Generation phase
    nwb_file = await self.agents["generation"].convert(
       request.data_path,
       metadata
    # 3. Evaluation phase
    validation = await self.agents["evaluation"].validate(nwb_file)
    # 4. TUIE monitoring (runs in parallel)
    metrics = await self.agents["tuie"].monitor_performance()
    # 5. Refinement if needed
    if validation.has_errors():
       nwb_file = await self.refine(nwb_file, validation.errors)
    return ConversionResult(
       nwb_file=nwb_file,
       validation=validation,
       metrics=metrics
```

5.3 Error Handling

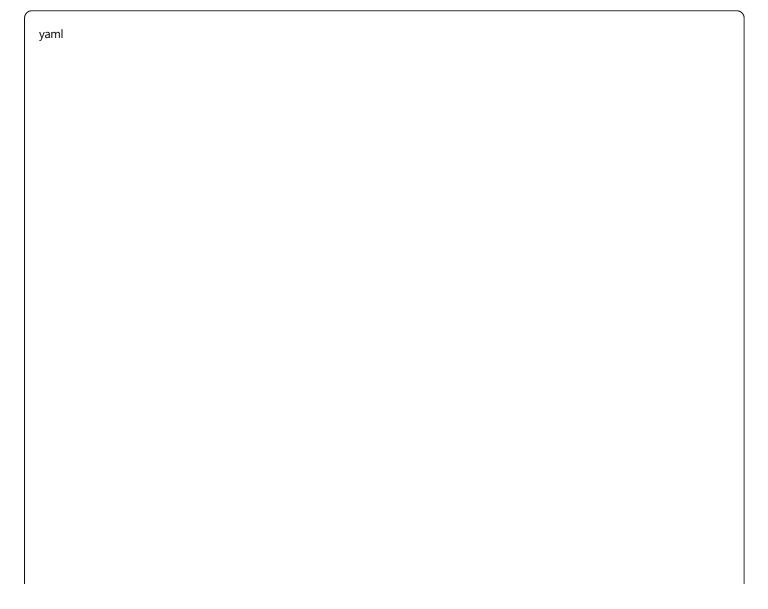
```
class MCPErrorHandler:

def __init__(self):
    self.retry_policy = ExponentialBackoff(
        max_retries=3,
        base_delay=1.0
)

async def handle_error(self, error: MCPError):
    if error.is_retryable():
        return await self.retry_with_backoff(error.request)
    elif error.is_critical():
        await self.alert_admin(error)
        raise CriticalPipelineError(error)
    else:
        return self.create_error_response(error)
```

6. Deployment Architecture

6.1 Docker Compose Configuration



version: '3.8' services: conversation-agent: build: ./agents/conversation environment: - MCP_SERVER_PORT=8001 - POSTGRES_CONNECTION= \${POSTGRES_CONNECTION} networks: - nwb-network generation-agent: build: ./agents/generation environment: - MCP_SERVER_PORT=8002 - NEUROCONV_VERSION=0.4.0 volumes: - ./data:/data networks: - nwb-network evaluation-agent: build: ./agents/evaluation environment: - MCP_SERVER_PORT=8003 - NWB_INSPECTOR_CONFIG=/config/inspector.yaml networks: - nwb-network tuie-agent: build: ./agents/tuie environment: - MCP_SERVER_PORT=8004 - MONITORING_ENABLED=true networks: - nwb-network orchestrator: build: ./orchestrator depends_on: - conversation-agent - generation-agent - evaluation-agent

- tuie-agent

- "8000:8000"

ports:



6.2 Kubernetes Deployment

```
apiVersion: apps/v1
kind: Deployment
metadata:
 name: nwb-conversion-pipeline
spec:
 replicas: 3
 selector:
  matchLabels:
   app: nwb-pipeline
 template:
  metadata:
   labels:
    app: nwb-pipeline
  spec:
   containers:
   - name: orchestrator
    image: nwb-pipeline/orchestrator:latest
    - containerPort: 8000
    env:
    - name: MCP_AGENTS
     value: "conversation,generation,evaluation,tuie"
   - name: conversation-agent
    image: nwb-pipeline/conversation-agent:latest
    ports:
    - containerPort: 8001
   # Additional containers for other agents
```

7. Monitoring and Observability

7.1 Metrics Collection

```
class MetricsCollector:
    def __init__(self):
        self.prometheus_client = PrometheusClient()
        self.metrics = {
            'conversion_duration': Histogram('conversion_duration_seconds'),
            'validation_errors': Counter('validation_errors_total'),
            'metadata_completeness': Gauge('metadata_completeness_ratio'),
            'agent_response_time': Histogram('agent_response_seconds')
      }

async def record_conversion(self, result: ConversionResult):
      self.metrics['conversion_duration'].observe(result.duration)
      self.metrics['validation_errors'].inc(len(result.errors))
      self.metrics['metadata_completeness'].set(result.metadata_score)
```

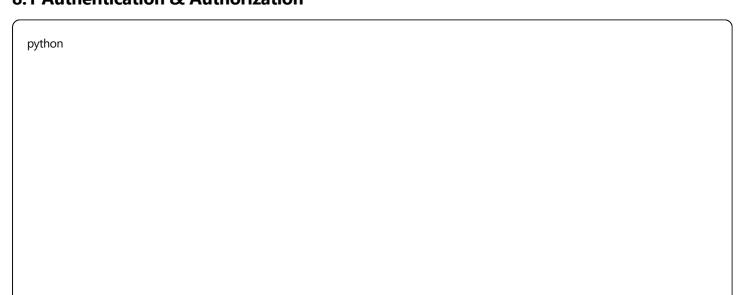
7.2 Logging Configuration



```
import structlog
logger = structlog.get_logger()
logging_config = {
  "version": 1,
  "disable_existing_loggers": False,
  "formatters": {
     "json": {
       "()": structlog.stdlib.ProcessorFormatter,
       "processor": structlog.processors.JSONRenderer(),
  "handlers": {
     "default": {
       "class": "logging.StreamHandler",
       "formatter": "json",
     },
     "file": {
       "class": "logging.handlers.RotatingFileHandler",
       "filename": "nwb_pipeline.log",
       "maxBytes": 10485760,
       "backupCount": 5,
       "formatter": "json",
```

8. Security Considerations

8.1 Authentication & Authorization



```
class SecurityManager:

def __init__(self):

self.auth_provider = OAuth2Provider()

self.rbac = RoleBasedAccessControl()

async def authenticate(self, token: str) -> User:

user = await self.auth_provider.verify_token(token)

permissions = self.rbac.get_permissions(user.role)

return AuthenticatedUser(user, permissions)

def authorize(self, user: User, action: str, resource: str) -> bool:

return self.rbac.check_permission(user, action, resource)
```

8.2 Data Encryption

```
class DataEncryption:
    def __init__(self):
        self.key_manager = KeyManager()

def encrypt_at_rest(self, data: bytes) -> bytes:
        key = self.key_manager.get_encryption_key()
        return encrypt(data, key)

def setup_tls(self):
    return {
        "cert_file": "/certs/server.crt",
        "key_file": "/certs/server.key",
        "ca_file": "/certs/server.key",
        "verify_mode": ssl.CERT_REQUIRED
    }
```

9. Testing Strategy

9.1 Unit Testing

```
class TestConversionAgent:

@pytest.fixture
def agent(self):
    return GenerationAgentMCP()

async def test_conversion_success(self, agent, sample_data):
    result = await agent.convert_dataset(sample_data)
    assert result.status == "success"
    assert Path(result.nwb_file_path).exists()

async def test_metadata_injection(self, agent, metadata):
    nwb_file = await agent.inject_metadata(metadata)
    assert nwb_file.subject.subject_id == metadata["subject_id"]
```

9.2 Integration Testing

```
class TestPipelineIntegration:
    async def test_end_to_end_conversion(self):
    # Setup test data
    test_data = create_test_dataset()

# Run full pipeline
    orchestrator = MCPOrchestrator()
    result = await orchestrator.process_conversion(test_data)

# Validate results
    assert result.validation.is_valid()
    assert result.metrics.performance_score > 0.8
```

10. Performance Optimization

10.1 Caching Strategy

```
class CacheManager:
    def __init__(self):
        self.redis_client = Redis()
        self.cache_ttl = 3600 # 1 hour

async def get_or_compute(self, key: str, compute_func):
        cached = await self.redis_client.get(key)
        if cached:
            return pickle.loads(cached)

result = await compute_func()
        await self.redis_client.setex(
            key,
            self.cache_ttl,
            pickle.dumps(result)
        )
        return result
```

10.2 Parallel Processing

```
python

class ParallelProcessor:

def __init__(self):
    self.executor = ProcessPoolExecutor(max_workers=4)

async def process_batch(self, files: List[str]):
    tasks = []
    for file in files:
        task = self.executor.submit(self.process_file, file)
        tasks.append(task)

results = await asyncio.gather(*tasks)
    return results
```

11. Maintenance and Updates

11.1 Version Management

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```
class VersionManager:
    def __init__(self):
        self.versions = {
            "pipeline": "1.0.0",
            "neuroconv": "0.4.0",
            "mcp_schema": "2.6.0",
            "mcp_protocol": "1.0"
        }

    def check_compatibility(self) -> bool:
        # Verify all components are compatible
        pass

    def upgrade_strategy(self, target_version: str) -> UpgradePlan:
        # Generate upgrade plan
        pass
```

11.2 Backup and Recovery

```
class BackupManager:
    def __init__(self):
        self.backup_storage = S3Storage()

async def backup_conversion(self, conversion_id: str):
    data = {
            "timestamp": datetime.now(),
            "input_data": self.get_input_data(conversion_id),
            "output_data": self.get_output_data(conversion_id),
            "metadata": self.get_metadata(conversion_id),
            "logs": self.get_logs(conversion_id)
        }

await self.backup_storage.upload(
            f'backups/{conversion_id}.tar.gz",
            self.compress(data)
        )
```

12. User Interface Specifications

12.1 Web UI Components

typescript

```
// React components for frontend
interface ConversionDashboard {
    sessionManager: SessionManager;
    metadataEditor: MetadataEditor;
    progressTracker: ProgressTracker;
    validationViewer: ValidationViewer;
    reportDownloader: ReportDownloader;
}

interface MetadataEditor {
    fields: MetadataField[];
    validation: ValidationRules;
    aiSuggestions: Suggestion[];
    onSave: (metadata: Metadata) => void;
}
```

12.2 CLI Interface

```
# Command-line interface
nwb-convert \
--input /path/to/data \
--output /path/to/output \
--metadata metadata,json \
--config config.yaml \
--validate \
--verbose

# Agent-specific commands
nwb-agent conversation --start --session-id abc123
nwb-agent generation --convert --input data.dat
nwb-agent evaluation --validate output
```