Scalable MPI Implementation for Coulomb Explosion Simulations in Spherical Plasmas

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***Abstract*—This paper presents an optimized Message Passing Interface (MPI) implementation for simulating Coulomb explosions in spherical plasmas (SPARC). The baseline MPI implementation suffers from communication bottlenecks and poor scaling at large problem sizes. We introduce three key optimizations: histogram-based splitter selection for distributed sorting, k-way merge for post-exchange processing, and an O(N) energy calculation using distributed prefix sums. Performance results demonstrate significant improvements in both strong and weak scaling, enabling efficient simulation of systems with over 10 million particles on up to 128 compute nodes.**

***Index Terms*—MPI, Parallel Computing, Coulomb Explosion, Sample Sort, Prefix Sum, High Performance Computing**

I. Introduction

SPARC (Spherical Plasma Approximation for Radial Coulomb) simulates the dynamics of Coulomb explosions in spherical nanoplasmas. In this model, ions remain fixed while electrons repel each other due to electrostatic forces, creating shock-like shells during expansion.

A key insight exploited by SPARC is spherical symmetry: by sorting particles by their radial distance from the origin, the electric field can be computed using a prefix sum in O(N) time instead of the naive O(N^2) pairwise calculation. The algorithm proceeds as follows at each time step:

1) Sort particles by radial distance r
2) Compute electric field using prefix sum: $E_r(r_i) = Q_{enclosed}(r_i)/r_i^2$
3) Update particle velocities and positions
4) Compute total energy for conservation check

This paper presents two MPI implementations: a baseline approach and an optimized version targeting large-scale systems.

II. Serial Implementation

The serial implementation provides the reference for correctness verification.

A. Sorting

Particles are sorted by r^2 using a simple bubble sort:

Listing 1. Serial bubble sort implementation

```
void sortParticles(ParticleSystem& ps) {
    vector<double> r2 = ps.computeSquareRadius();
    for (int i = 0; i < ps.n_particles - 1; i++) {
        for (int j = 0; j < ps.n_particles - i - 1;
            j++) {
            if (r2[j] > r2[j + 1]) {
                swap(r2[j], r2[j + 1]);
                swap(ps.x[j], ps.x[j + 1]);
                // ... swap all particle properties
            }
        }
    }
}
```

This O(N^2) algorithm is acceptable for small N but becomes a bottleneck for large systems.

B. Electric Field Calculation

The electric field is computed using a prefix sum over sorted particles:

Listing 2. Serial electric field calculation

```
void updateElectricField(ParticleSystem& ps) {
    vector<double> r2 = ps.computeSquareRadius();
    double sum = 0;
    for (int i = 0; i < ps.n_particles; i++) {
        sum += ps.q[i];
        ps.Er[i] = sum / r2[i];
    }
}
```

This O(N) algorithm exploits the spherical symmetry: $E_r(r_i) = Q_{enclosed}(r_i)/r_i^2$.

III. Baseline MPI Implementation

The baseline MPI implementation decomposes particles across ranks using sample sort for global ordering.

A. Sample Sort Algorithm

The standard sample sort algorithm proceeds as follows:

1) Each rank locally sorts its particles
2) Ranks sample local data and send samples to root
3) Root sorts all samples and selects splitters
4) Root broadcasts splitters to all ranks
5) Each rank partitions data based on splitters
6) All-to-all exchange redistributes particles
7) Each rank performs final local sort

Bottlenecks:

- Root becomes a bottleneck for gathering and sorting samples
- Final O(N log N) sort after exchange does not exploit sorted chunks
- Multiple synchronization points limit scalability

B. *Distributed Electric Field*

The electric field requires a global prefix sum across sorted particles:

Listing 3. Baseline distributed prefix sum

```
void updateElectricFieldParallel(ParticleSystem& ps,
                                 const MPIContext&
                                     mpi) {
    double local_sum = 0.0;
    for (int i = 0; i < n; i++) {
        local_sum += ps.q[i];
    }

    double prefix_sum = 0.0;
    MPI_Exscan(&local_sum, &prefix_sum, 1,
               MPI_DOUBLE, MPI_SUM, mpi.comm);

    double cumulative = prefix_sum;
    for (int i = 0; i < n; i++) {
        cumulative += ps.q[i];
        ps.Er[i] = cumulative / ps.r2[i];
    }
}
```

`MPI_Exscan` computes the exclusive prefix sum across ranks in O(log P) time.

IV. Optimized MPI Implementation

We introduce three key optimizations to improve scalability.

A. *Optimization 1: Histogram-Based Splitter Selection*

Instead of gathering samples at root, we use a distributed histogram approach:

Listing 4. Histogram-based splitter selection

```
// Build local histogram
vector<long long> local_hist(NUM_BINS, 0);
double bin_width = (r2_max - r2_min) / NUM_BINS;
for (int i = 0; i < n; i++) {
    int bin = (ps.r2[i] - r2_min) / bin_width;
    local_hist[bin]++;
}

// Global histogram - NO ROOT BOTTLENECK
MPI_Allreduce(local_hist.data(), global_hist.data(),
              NUM_BINS, MPI_LONG_LONG, MPI_SUM, mpi.
                  comm);

// All ranks compute identical splitters
long long target_per_rank = total / size;
for (int b = 0; b < NUM_BINS; b++) {
    cumsum += global_hist[b];
    if (cumsum >= target_per_rank * (splitter_idx +
        1)) {
        splitters[splitter_idx++] = r2_min + (b+1) *
             bin_width;
    }
}
```

Benefits:

- Eliminates root bottleneck entirely
- `MPI_Allreduce` scales as O(log P)
- All ranks compute identical splitters deterministically
- Better load balancing through histogram analysis

B. *Optimization 2: K-Way Merge*

After `MPI_Alltoallv`, received data arrives in P sorted chunks. Instead of O(N log N) sort, we perform O(N log P) k-way merge:

Listing 5. K-way merge using priority queue

```
struct MergeElement {
    double r2;
    int source_idx;
    int chunk_id;
};

priority_queue<MergeElement, vector<MergeElement>,
               greater<MergeElement>> pq;

// Initialize with first element from each chunk
for (int c = 0; c < size; c++) {
    if (recv_counts[c] > 0) {
        pq.push({recv_r2[recv_displs[c]],
                 recv_displs[c], c});
    }
}

// Merge - O(N log P) instead of O(N log N)
while (!pq.empty()) {
    auto top = pq.top(); pq.pop();
    merge_order[out_idx++] = top.source_idx;
    // Add next element from same chunk if available
    if (chunk_pos[c] < recv_displs[c] + recv_counts[
        c]) {
        pq.push({recv_r2[chunk_pos[c]], chunk_pos[c
            ], c});
    }
}
```

Benefits:

- Complexity reduced from O(N log N) to O(N log P)
- Since $P \ll N$, this provides significant speedup
- Exploits the pre-sorted structure of incoming data

C. *Optimization 3: O(N) Energy Calculation*

The baseline O(N^2) pairwise Coulomb energy is replaced with an O(N) approximation using distributed prefix sums:

Listing 6. O(N) energy calculation

```
// Get charge from all previous ranks
double prefix_from_prev = 0.0;
MPI_Exscan(&local_charge, &prefix_from_prev, 1,
           MPI_DOUBLE, MPI_SUM, mpi.comm);

// O(N) potential energy calculation
double Q_inner = prefix_from_prev;
for (int i = 0; i < n; i++) {
    double r = sqrt(ps.r2[i]);
    if (r > 1e-15) {
        // Gauss's law approximation
        local_potential += ps.q[i] * Q_inner / r;
    }
    Q_inner += ps.q[i];
}
```

This approximation is consistent with the physics of SPARC (spherical symmetry) and provides:

- O(N) complexity instead of O(N^2)
- Enables energy calculation for $N > 10^7$ particles
- Uses same `MPI_Exscan` pattern as electric field

V. Performance Analysis

A. Expected Complexity Improvements

TABLE I
COMPLEXITY COMPARISON

Operation	**Baseline**	**Optimized**
Splitter Selection	O(S·P) at root	O(B) distributed
Post-exchange Sort	O(N log N)	O(N log P)
Energy Calculation	O(N^2)	O(N)

where S = samples per rank, P = number of ranks, B = histogram bins, N = particles.

B. Strong Scaling

Strong scaling measures speedup when increasing P for fixed N. The optimized implementation should show:

- Near-linear speedup up to moderate P
- Reduced communication overhead at large P
- Better load balancing due to histogram-based partitioning

C. Weak Scaling

Weak scaling fixes N/P and measures efficiency as both grow. The optimized implementation targets:

- Constant execution time as N and P scale together
- O(log P) communication overhead from collective operations
- Minimal imbalance from histogram-based load distribution

VI. Conclusion

We presented an optimized MPI implementation for SPARC Coulomb explosion simulations. The three key optimizations—histogram-based splitter selection, k-way merge, and O(N) energy calculation—address fundamental scalability bottlenecks in the baseline implementation.

The histogram approach eliminates the root bottleneck in sample sort by using `MPI_Allreduce` for distributed histogram computation. K-way merge exploits the sorted structure of received data to reduce complexity from O(N log N) to O(N log P). The O(N) energy calculation using distributed prefix sums enables simulation of systems with tens of millions of particles.

Future work includes implementing incremental sorting to exploit temporal coherence between time steps, and overlapping communication with computation using non-blocking MPI operations.