Using Shared Arrays in Message-Driven Parallel Programs

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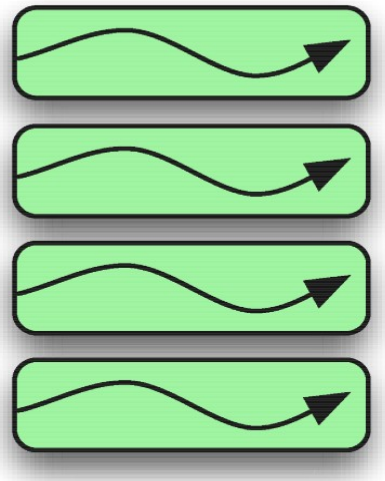
Object-Based, Message Driven

- All data owned by objects
  - Locality
  - Virtualization & Migratability
- Communication is explicit & directed

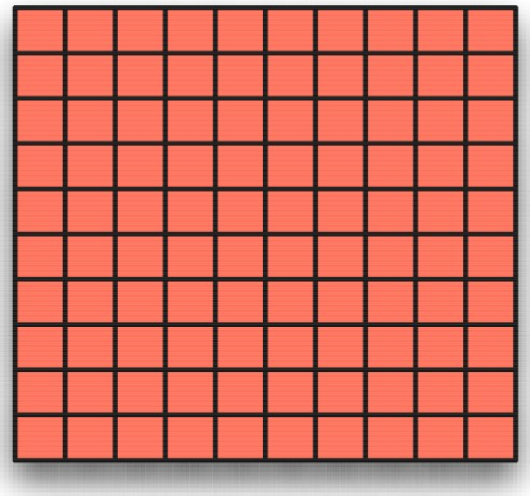
Why Shared Arrays

- Many units accessing common data
- No 'owner'
- Irregular or unpredictable communication

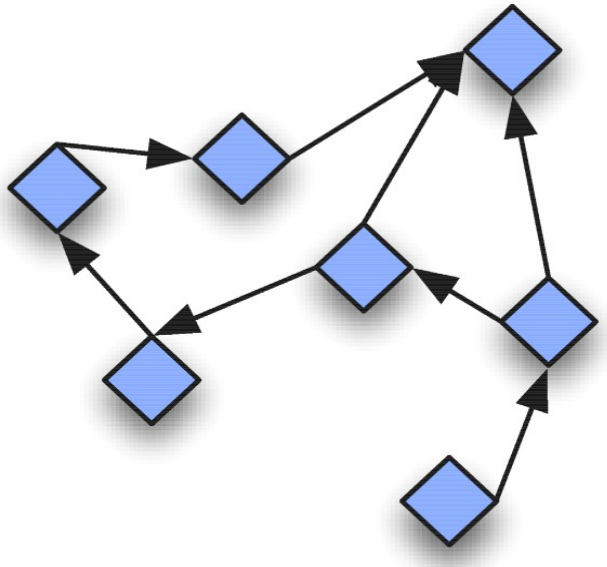
Shared Arrays in Charm++



Client Threads

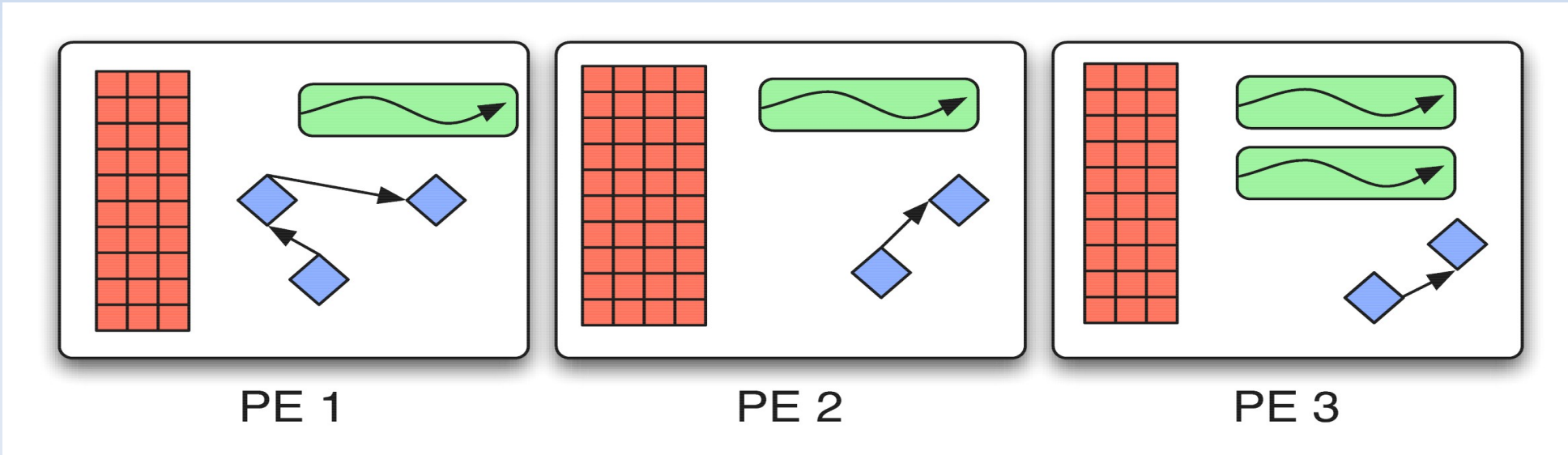


MSA



Message-driven Objects

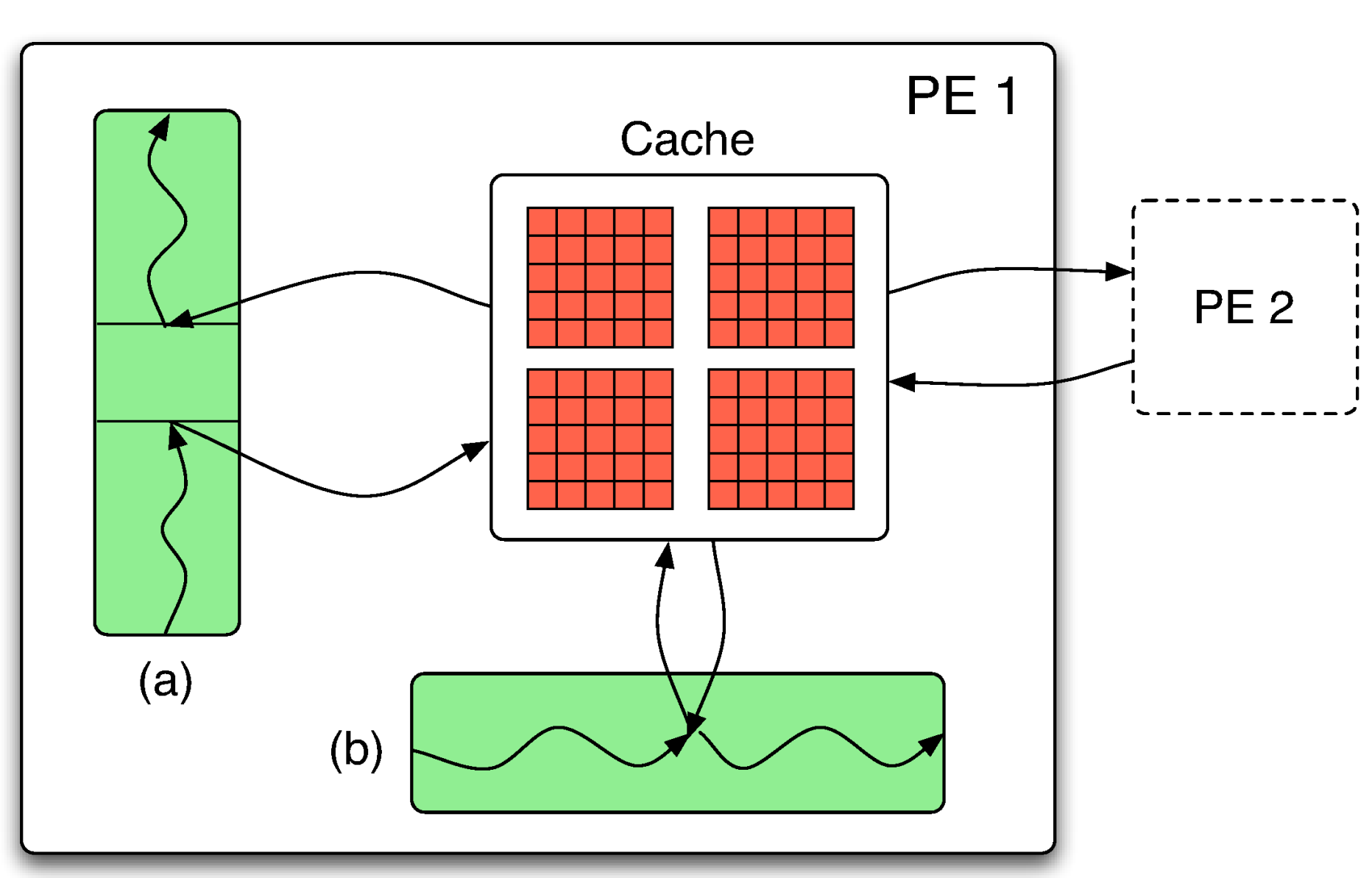
Shared Arrays in Charm++



Phases

- Many applications are 'nice'
- All write, all read, repeat
- Utility?

Caching



Mode-Based Safety

- Read-only
- Exclusive Write
- Accumulate

Mode-Based Safety

- Typed Handles

Read r;
Accum a;

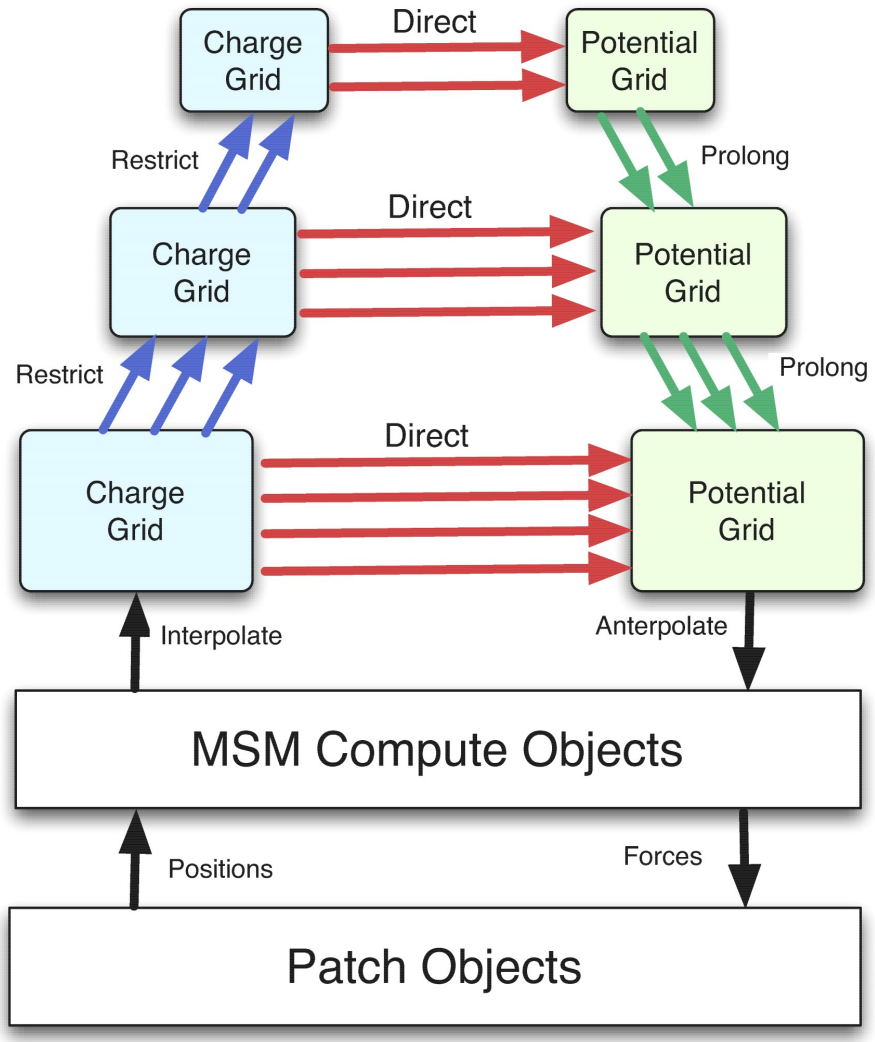
```
do {
  double minDistance = distance(r, curSeed);
  for (int i = 0; i < numClusters; ++i) {
    double d = distance(r, i);
    if(d < minDistance) {
     minDistance = d;
     newSeed = i;
    }
  }
  // Start accumulating new positions
  a = r.syncToExcAccum();
  // Each PE adds itself to its new seed
  for (int i = 0; i < numMetrics; ++i)
    a(newSeed, i) += metrics[i];

  // Update membership and change count
  a(newSeed, numMetrics) += 1;
  if (curSeed != newSeed)
    a(0, numMetrics+1) += 1;
  curSeed = newSeed;

  // Put the array in Read mode
  r = a.syncToRead();
} while(r(0, numMetrics+1) > 0);
```

- Synchronization couples very tightly
- Hurts modularity
- Constrained control flow can hurt performance

- Messaging to the rescue!




```
void Driver::step() {
    // Phase 1: Atoms to Charge grid
    computes.contributeCharges(Acharges);
    direct.dummySync(Acharges);
    energy.dummySync(Acharges);
    inner[1].syncRestriction(Acharges);
    gread Rcharges = Acharges.syncToRead();

    // Phase 2: Charge grid to Potential grid
    direct.calculate(Rcharges, Apotentials);
    inner[1].calculate(Rcharges, Apotentials);

    computes.dummySync(Apotentials);
    energy.dummySync(Apotentials);
    gread Rpotentials = Apotentials.syncToRead();

    // Phase 2.5: Potential energy
    if (calc_potential_energy)
      energy.calculate(Rcharges, Rpotentials);

    computes.dummySync(Rcharges);
    Acharges = Rcharges.syncToEAccum();

    // Phase 3: Potential grid to Atoms
    computes.readPotentials(Rpotentials);
    direct.dummySync(Rpotentials);
    inner[1].syncProlongation(Rpotentials);
    Apotentials = Rpotentials.syncToEAccum();
}
```

```
entry void MSMCompute::step() {
  when interact(ParticleDataMsg *msg),
       contributeCharges(Accum charges) {
    particles = msg;
    computeChargeGrid(charges);
    charges.syncDone();
  }

  when readPotentials(Read potentials) {
    forceMsg = new ParticleForceMsg;
    computeForces(potentials, forceMsg);
    patch.receiveForces(forceMsg);
    potentials.syncDone();
    delete particles;
  }
}
```

```
entry void Energy::calculate(Read charges,
                             Read potentials)
{
  double u = 0.0;

  for(int i = 0; i < grid_x[0]; ++i)
    for(int j = 0; j < grid_y[0]; ++j)
      for(int k = 0; k < grid_z[0]; ++k)
       u += charges(i,j,k) * potentials(i,j,k);

  CkPrintf(”MSM Potential: %f\n”, u);

  charges.syncDone();
  potentials.syncDone();
}
```

Conclusion

- In progress:
  - QM/MM
  - Migratability
- Questions?