The X10 language supports distributed arrays of arbitrary shape and distribution, allowing succinct expression of complex scientific applications. We have extended X10's parallel language constructs to implement efficient high-level operations over distributed arrays.

### Efficient distributed parallel loops

X10 supports distributed parallel loops with the `ateach` construct. Our proposed enhancement to the X10 compiler transforms `ateach` to a tree-based broadcast/reduce communication pattern. We used our enhanced `ateach` to scale Fast Multipole Method (molecular dynamics), Smooth Particle Mesh Ewald and Hartree Fock (quantum chemistry) codes to large numbers of processors.

```java
// Particle Mesh Ewald - get direct energy
val directEnergy = finish(SumReducer()) {
    ateach((x, y, z) in subCells) {
        val cellEnergy = ...
        offer cellEnergy;
    }
};
```

### Extending the X10 array library

**Ghost regions**

Ghost regions are a common feature in distributed structured grid applications. A ghost region is a local read-only copy of remotely-held boundary data; processes coordinate to exchange ghost data many times during a computation. We extend X10 distributed arrays so ghost data are accessed by the same methods as locally held data. Ghost region updates are implemented using active messages with only local synchronization between neighboring processors, eliminating the need for a global barrier. We use ghost regions to implement molecular dynamics and fluid dynamics simulations on regular grids.

```java
// at each X10 place
distArray.sendGhosts();
distArray.waitForGhosts();
```

**Periodic boundary conditions**

Periodic (wrapped) boundary conditions are common in molecular dynamics and fluid dynamics simulations. Supporting PBCs in the array library frees the programmer from managing modular indexing, and allows for efficient stencil operations. We used the enhanced array library to implement a periodic Fast Multipole Method and the Smooth Particle Mesh Ewald method for electrostatic interactions in periodic molecular simulations.

All codes available as free software in the ANUChem suite of computational chemistry codes in X10: http://cs.anu.edu.au/~Josh.Milthorpe/anuchem

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