

## **Particle-Based Applications**

Particle-based simulation approaches are ubiquitous in computational science and engineering. The “particles” may represent, for example, the atomic nuclei of quantum and classical molecular dynamics methods or gravitationally interacting bodies or tracer particles in N-body simulations. In each case, every particle interacts with its environment by direct particle-particle interactions at shorter ranges and/or the particle-mesh interactions between a particle and a local field that is set up by longer range effects.

The Co-design Center for Particle Applications (**CoPA**) is addressing the challenges for particle-based applications to run on upcoming exascale computing architectures by partnering with ECP applications teams to create co-designed numerical recipes for particle-based methods: short-range particle-particle interactions (e.g., those which often dominate molecular dynamics methods), long-range particle-particle (e.g., electrostatic and gravitational) interactions, particle-in-cell methods, and linear-scaling electronic structure and quantum molecular dynamics algorithms.

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