

# SI2-SSE: Expanding the Scope of Materials Modeling with EPW Software

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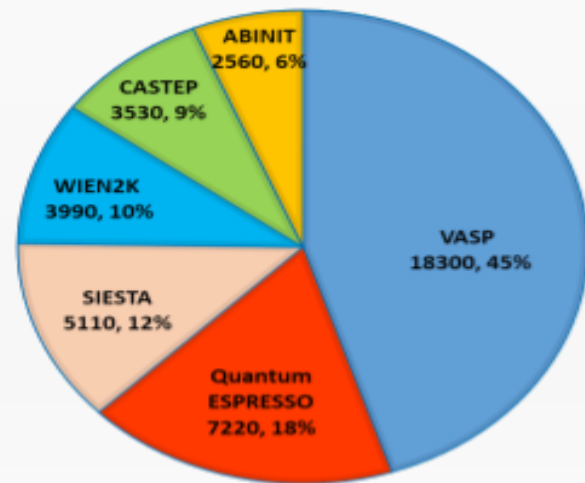
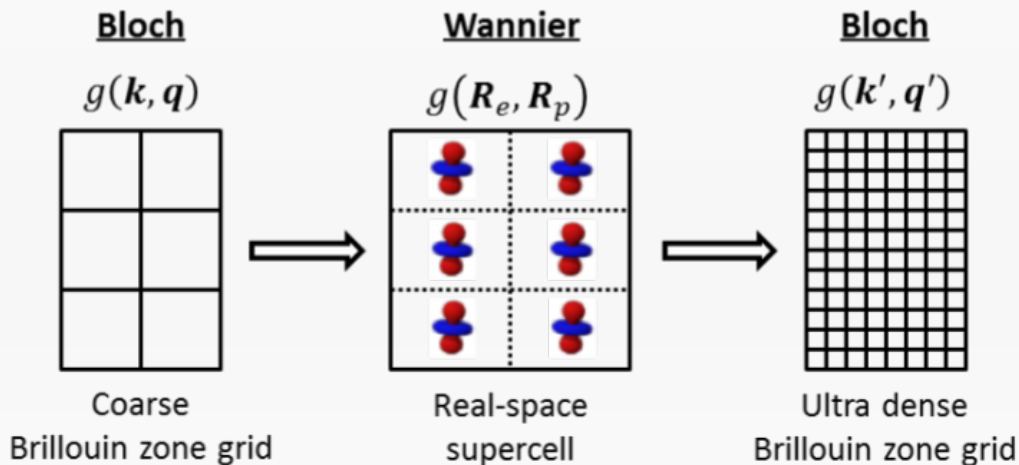
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# Methodology and Usage

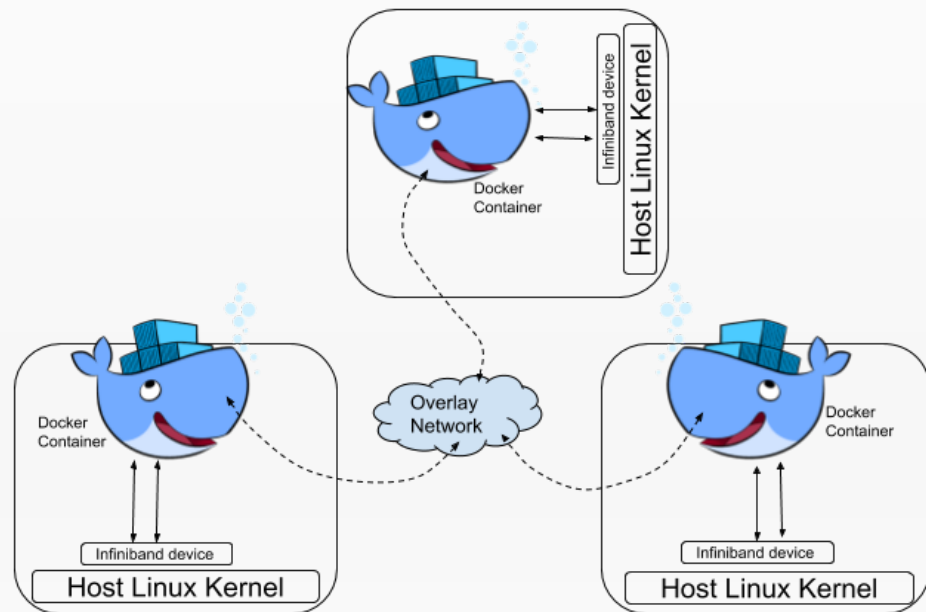
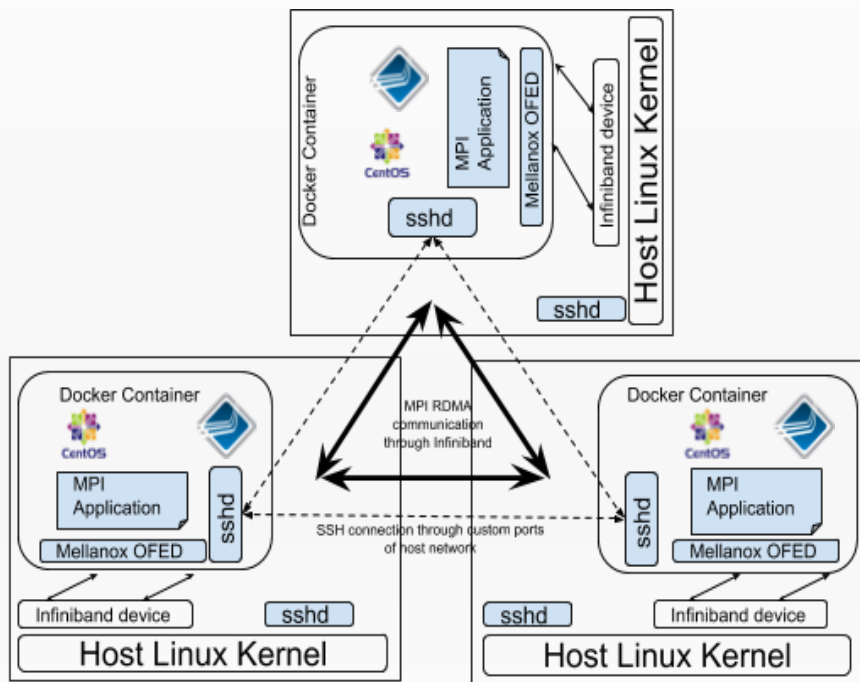
- EPW is an open-source Fortran90/MPI code that uses density-functional perturbation theory and maximally localized Wannier functions
- EPW provides unprecedented levels of accuracy and efficiency in calculations of materials properties defined by the interaction between electrons and atomic vibrations (i.e., electron-phonon interactions)
- Electron-phonon interactions are critical for understanding and designing electronic materials and devices (e.g., semiconductors, superconductors, and thermoelectrics).

## Accuracy boost workflow in EPW



# Containers, Cloud, and Scientific Codes

- Apache Mesos framework, Scylla, that leverages Docker Swarm for orchestration of containerized scientific jobs.
- Developed a policy driven approach to manage CPU, memory, and networking resources more efficiently across VMs allocated on the Chameleon cloud.



# Next Steps

- Develop and implement accurate and robust software elements to model spin-dependent materials properties from first principles
- Implement adaptive schemes for Brillouin zone integration
- Enable EPW usage with existing and emerging large-scale infrastructures such as NSF Clouds
- Develop Gateway Interfaces to ease usage of EPW
- Expand documentation, end user support, example library, and automated non-regression testbed