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Simple use of Intel® oneMKL for high performance

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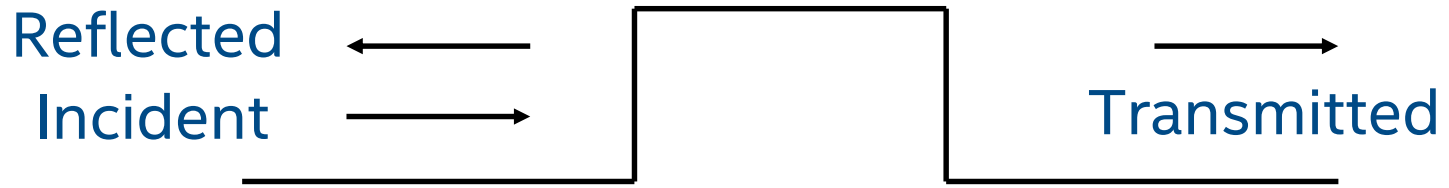
Motivation

- Optimized math libraries play a significant role in a very large number of High Performance Computing (HPC) applications.
- Excellent way to get a good degree of performance portability with relatively limited effort in many cases.
- Application layers can be designed to enable developers to easily adopt native math libraries on new platforms.
- Are there algorithms which are particularly well suited to leverage the benefits provided by optimized math libraries?
  - If so, can these algorithms be applied in a wide variety of contexts?

Case study: Wave Scattering

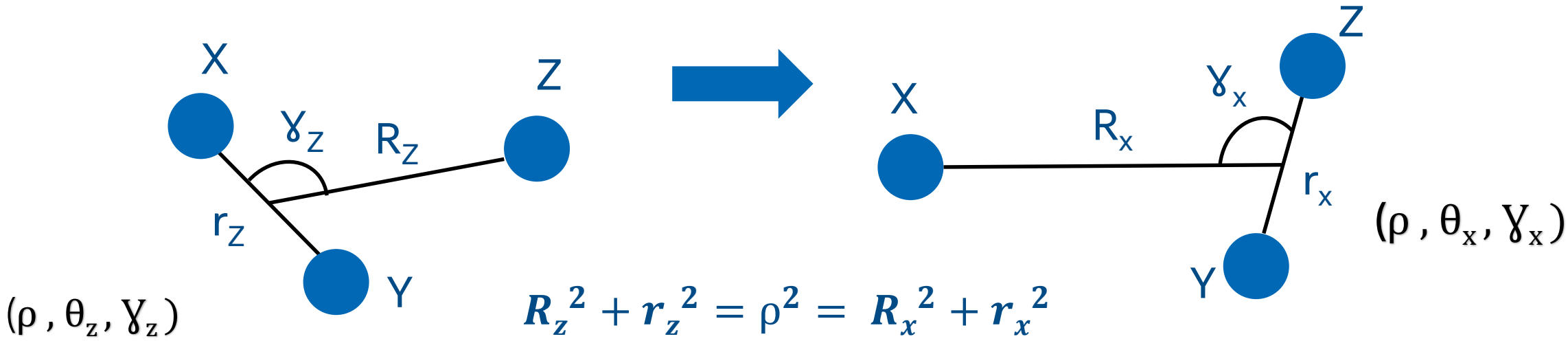
- Reflection/Transmission problems in Electromagnetics, Quantum Mechanics, Seismology
- In 1D these boundary value problems can be solved in segments
  - The propagations can be written as a sequence of small matrix multiplications (explicit) or inversions (implicit)



- In 2D or 3D, the propagations become a series of large matrix multiplications or matrix inversions (LU factorizations)

Specific cases

- Historical inspiration:
  - "On the intensity of the light reflected from or transmitted through a pile of plates" by George Gabriel Stokes, Proc of Royal Soc London, 11, December 31st 1862.
- Less direct application, the Quantum 3-Body Problem



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Conclusions

- A relatively large number of problems can efficiently be represented as sequences of matrix multiplications or inversions in relatively simple loop structures.
- These types of problems are ideally suited to achieve a good degree of performance portability across architectures provided optimized math libraries exist on these architectures.
- Tests show that Intel oneMKL is a good choice for these kinds of problems on commonly available Intel® architecture platforms.

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