Developing exascale spectral/hp element tools for fusion applications

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We are developing efficient high-order spectral/hp element solvers and proxyapps for the NEPTUNE project, examining the numerical and computational performance for testbed fusion applications. In particular we are:

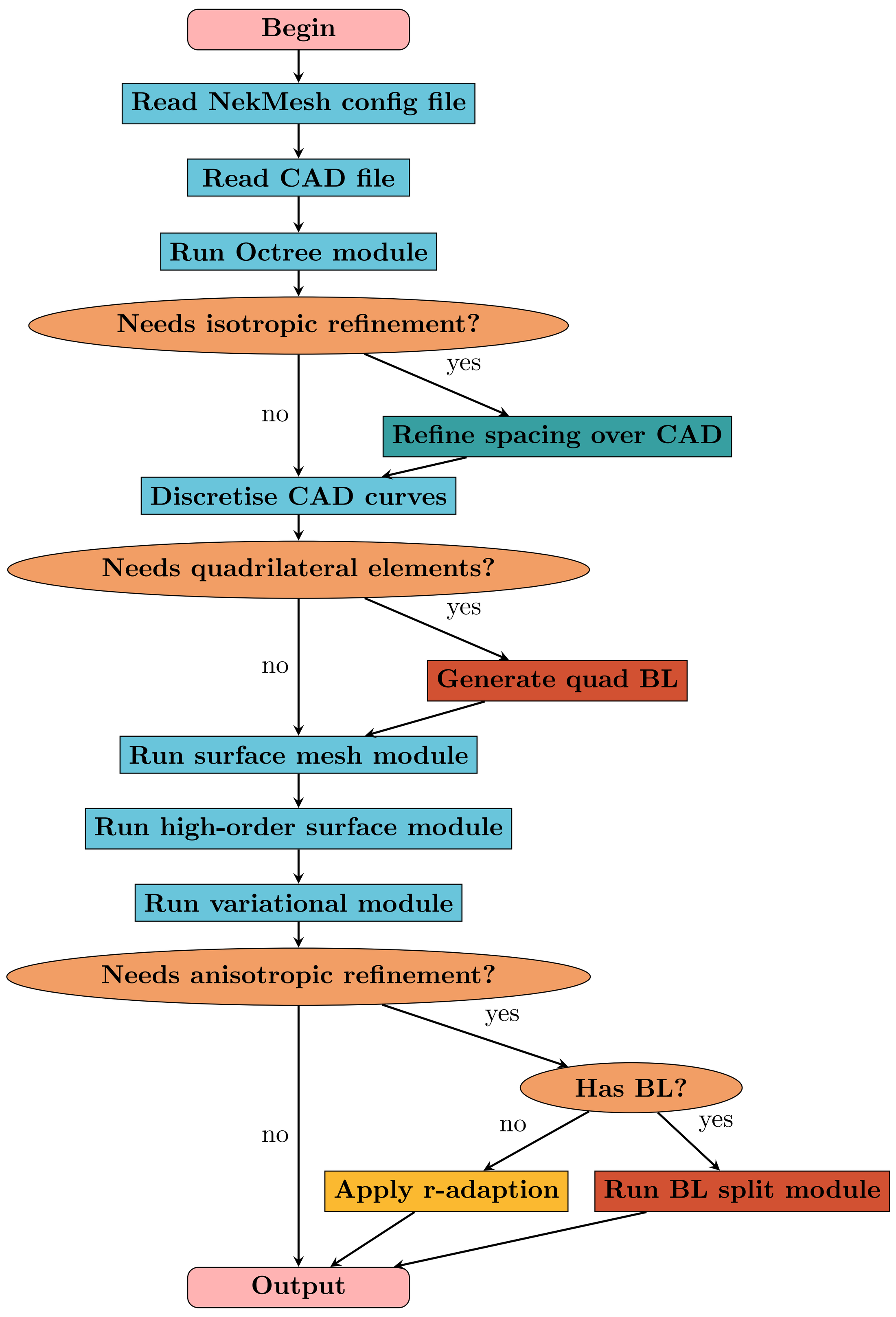
- **generating high-quality meshes that are suited to the highly anisotrotropic physics found in these simulations;**
- **developing high-performance execution kernels for the heterogeneous hardware that powers exascale computing.**

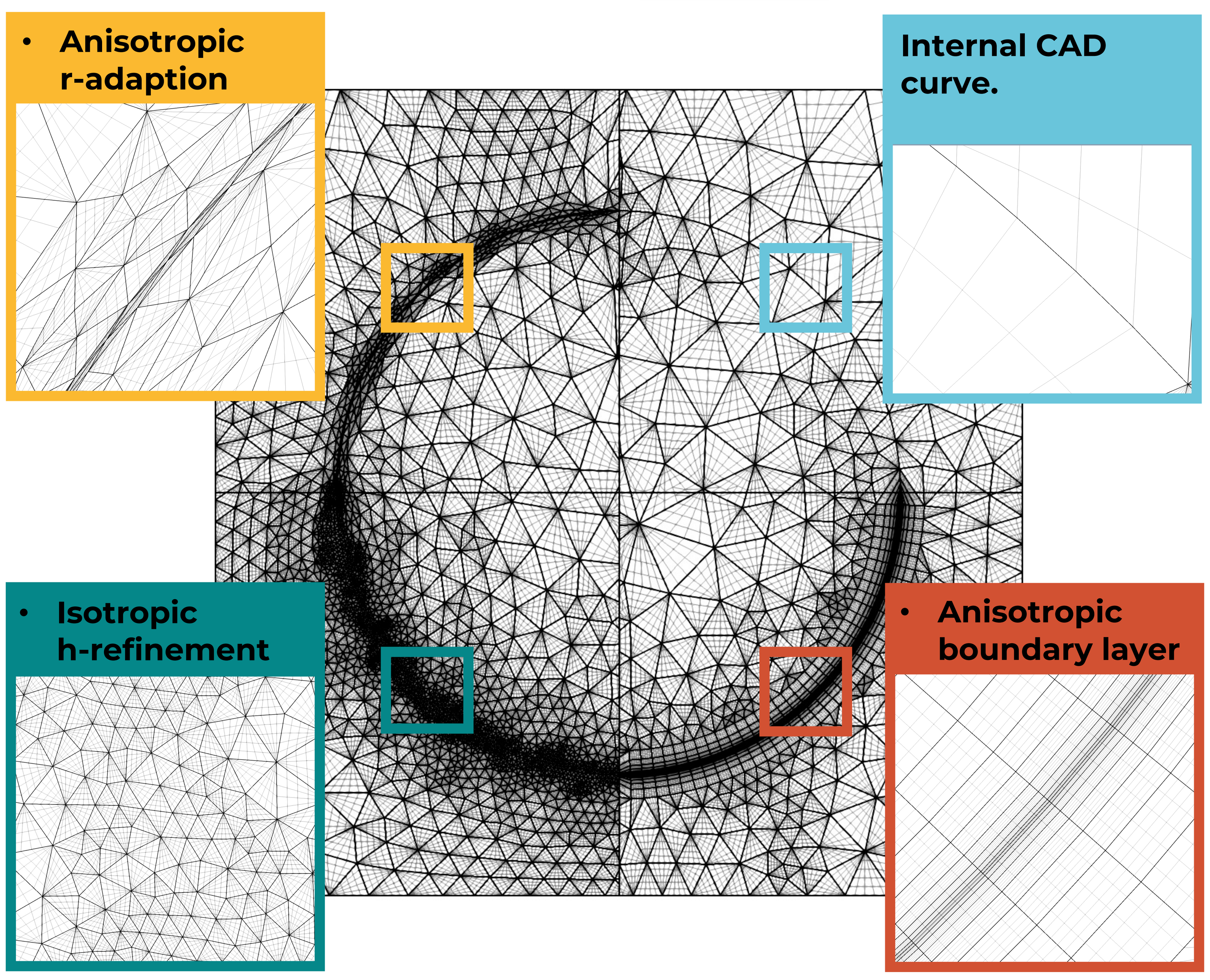
Anisotropic high-order mesh generation for internal flow features using embedded CAD curves

High-order simulations require **high-order meshes** which conform to the underlying geometry, including curving elements to align with this geometry. In this project we have been extending our capabilities to resolve **geometry-interior features** such as the plasma separatrix found in a tokamak's interior.

The flowchart demonstrates the bottom-up approach taken in our mesh generator **NekMesh** to generate high-order meshes. These have been extended to resolve these features, by using interior CAD geometries to conform and refine the mesh with the flow structures. This includes:

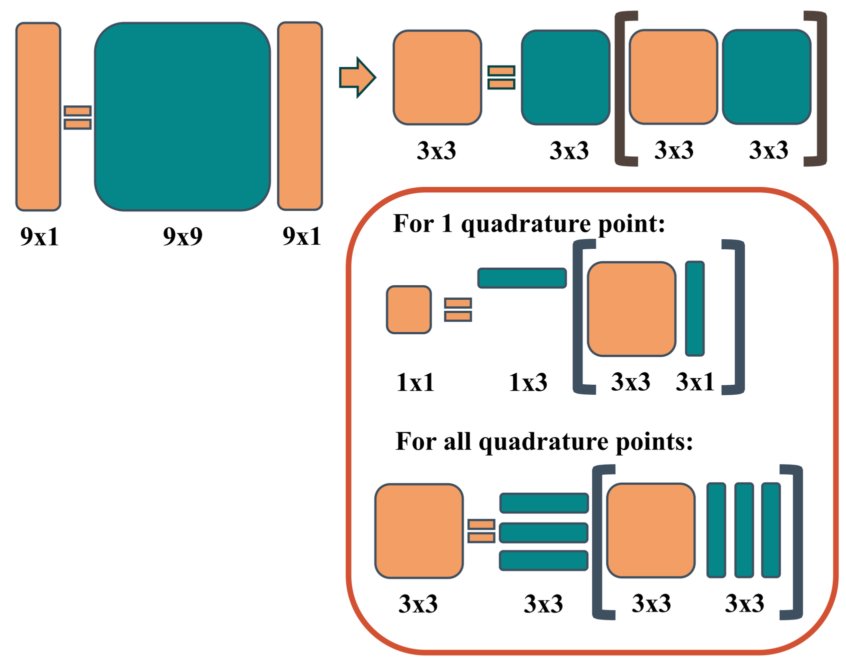
- Isotropic *h*-refinement;
- Anisotropic mesh refinement using *r*-adaptation;
- Quadrilateral anisotropic boundary layer (BL) meshes generated on both sides of the CAD geometry.



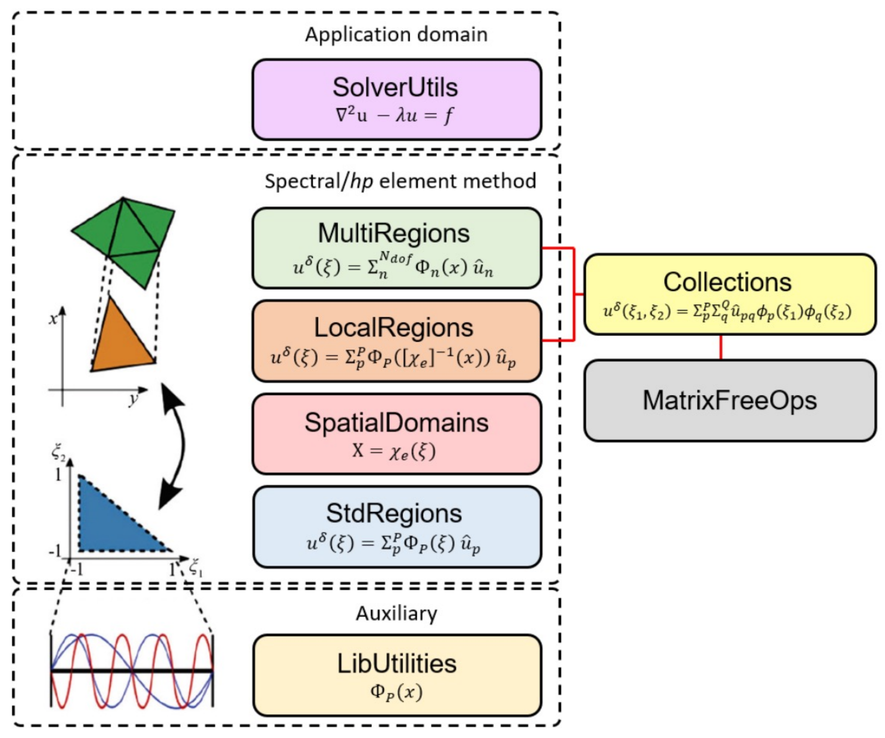


Helmholtz matrix-free operators in Nektar++

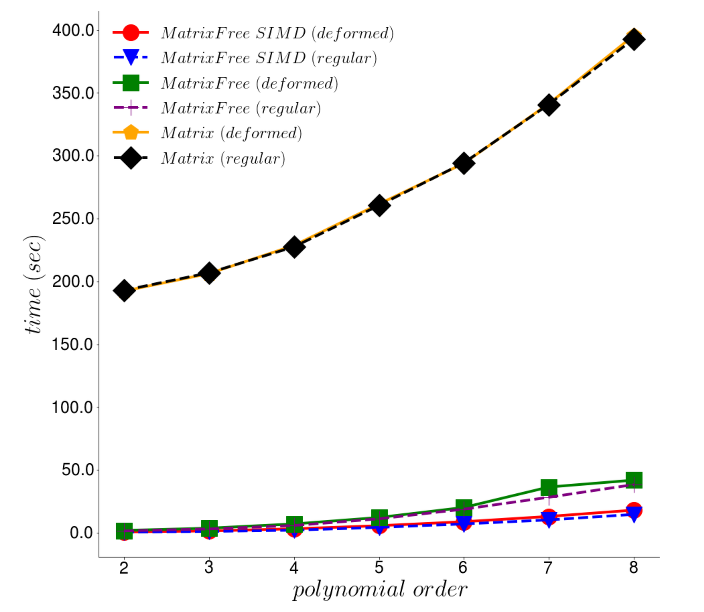
We have developed efficient finite element operators using **matrix-free evaluations** of the block inner-product, derivative and interpolation kernels from which they are constructed. These target **x86, ARM and GPU** architectures, ensuring use of SIMD vectorization through templating and data interlacing of elemental data. We leverage **sum factorization** for reduced operator complexity & improved throughput.



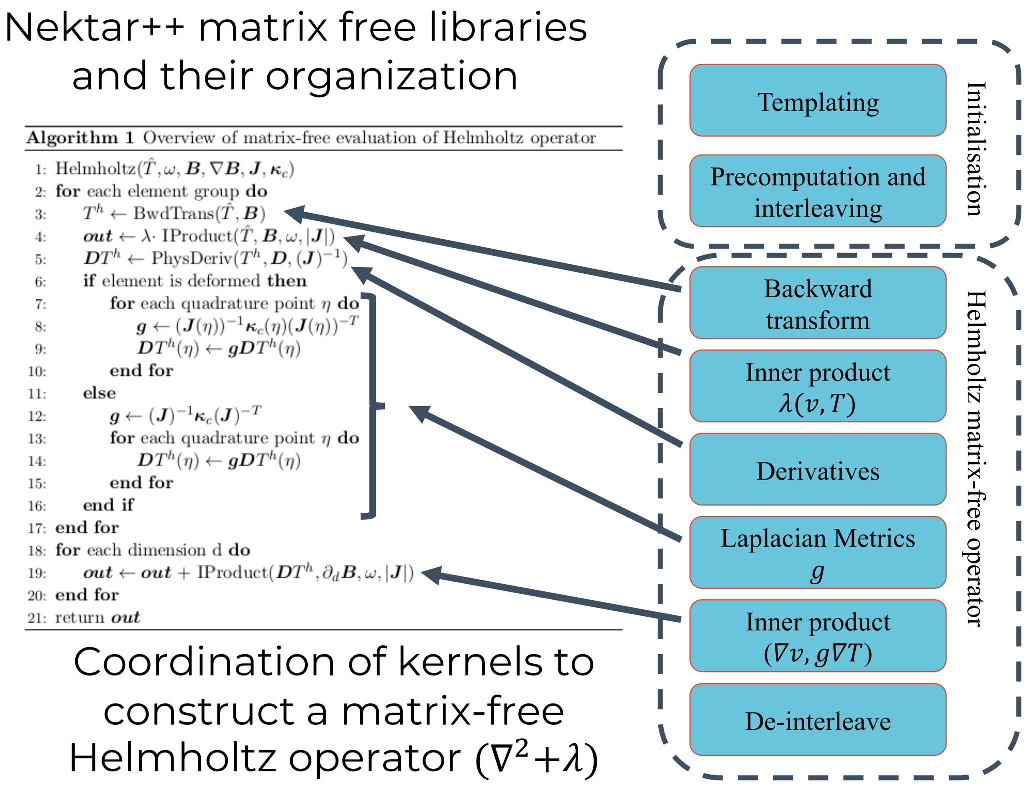
Sum-factorization (backward transformation) improves operator complexity and efficiency



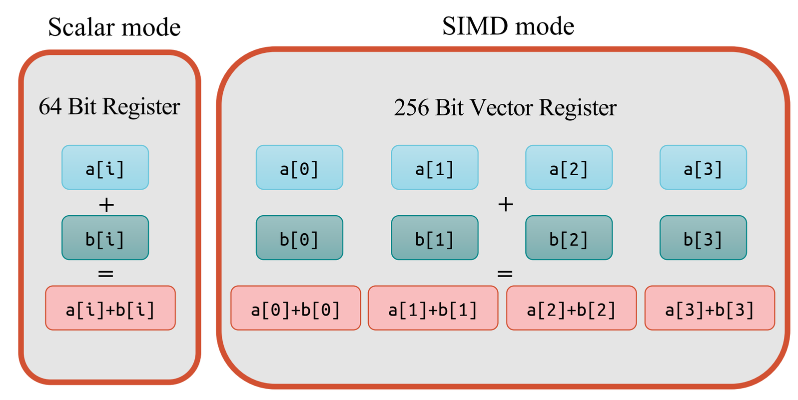
Nektar++ matrix free libraries and their organization



Performance of CPU Helmholtz matrix-free operator



Coordination of kernels to construct a matrix-free Helmholtz operator ($\nabla^2+\lambda$)

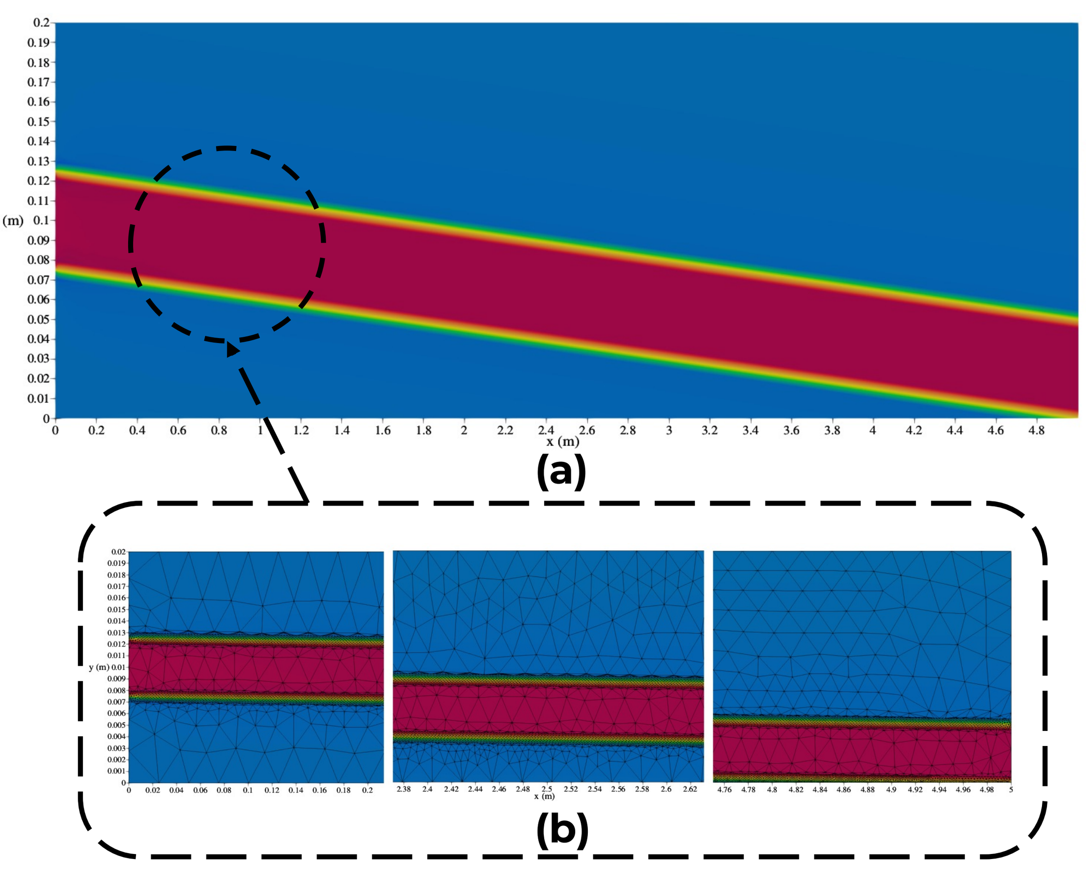


Single-instruction, multiple-data (SIMD) intrinsics are used to ensure optimal performance of kernel evaluations

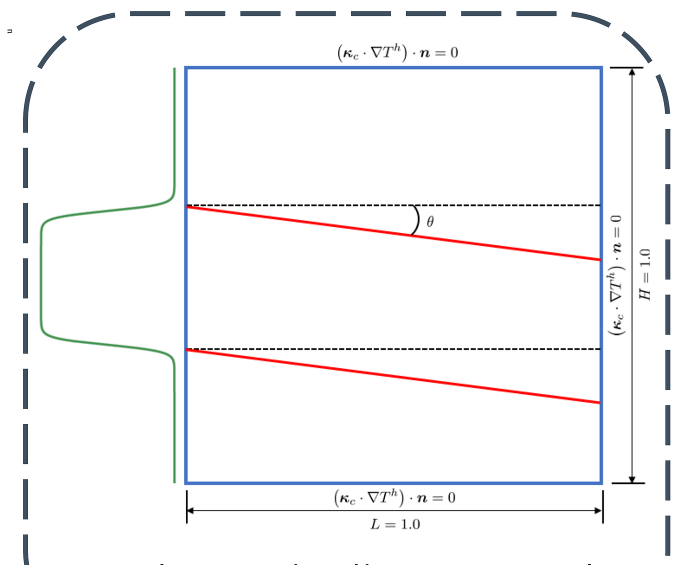
Thermal conduction of anisotropic magnetised plasma simulation

We have used this infrastructure to develop proxyapps for NEPTUNE use cases, such as a highly anisotropic heat transport problem:

$$\frac{3}{2}n\frac{\partial T}{\partial t} = \nabla \cdot \begin{bmatrix} ((\kappa_{\parallel}-\kappa_{\perp})cos^2\theta+\kappa_{\perp})\partial_x T + ((\kappa_{\parallel}-\kappa_{\perp})cos\theta sin\theta)\partial_y T \\ ((\kappa_{\parallel}-\kappa_{\perp})cos\theta sin\theta)\partial_x T + ((\kappa_{\parallel}-\kappa_{\perp})cos\theta sin\theta)\partial_y T \end{bmatrix} + Q$$



Snapshot of the thermal conduction of magnetized plasma: **(a)** strong thermal anisotropy along the magnetic field in plasma and **(b)** the refined mesh along scrape-off layer



Schematic diagram and boundary conditions

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