Parallel Cell-Based Finite element test with Dealii

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Outline

Punchline

Want to discretize some continuous differential operator
Typical Finite element method

- Construct sparse matrix
- Solve using linear algebra engines

Finite element method

Parameterize geometry

- Divide structure in simple (unstructured) cells
- Enables us to perform integrations and define basis functions

Build basis functions (polynomials on the cells)

- Continuous
- Simple derivatives
- Easy to integrate over cells

Solve $Lu = b$ for some sparse matrix L

Matrix-free vs sparse matrix

IDEA: Main memory is bottle neck for scientific computing (big grids which do not fit in cache) - Substitute looking up matrix elements in memory by re-computing them. Access the matrix by evaluating matrix-vector products.
Don't assemble a global sparse matrix Instead only store

- the unit cell shape function information
- the enumeration of the dofs (vertices of mesh)
- transformation from unit cell to real cell

Arrange operations such that successive Matrix-Vector operations are performed $\rightarrow$ less memory transfer during computations

Matrix-free class in Dealii

MPI parallelization on clusters of distributed nodes

- Domain decomposed into subdomains of equal size and assigned to individual processors.
- Each processor holds a coarse mesh on the entire domain
- Data associated to dofs on the subdomain boundaries are available to all processors involved.

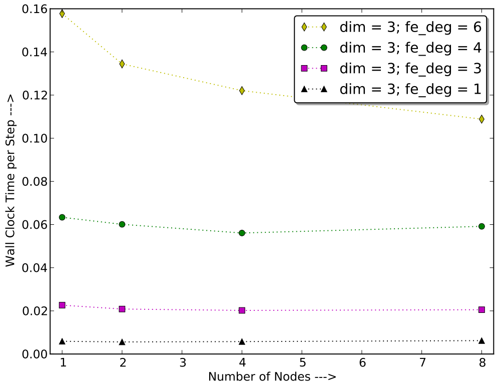
Thread parallelization scheduled by Threading Building Blocks library

- Subdivide cells into subdomains with precomputed neighbor relations
- Use Intel Threading Building Blocks to schedule tasks dynamically in such a way that no neighboring cells are worked on simultaneously. (Color graph problem: No two adjacent cells with the same color).
- Algorithm:
    1. Partition domain such that cells belonging to partition k at most overlap with partitions k-1,k,k+1 so that all even/odd partitions are independent
    2. Within each partition subdivide the cells following the same strategy as in part (1)

Vectorization by clustering of two or more cells into a SIMD data type for operator application

- Custom vectorization within the CPU (SIMD)
- Operations are typically the same on all cells

Scaling with number of nodes


dim = 3; fe_deg = 6
dim = 3; fe_deg = 4
dim = 3; fe_deg = 3
dim = 3; fe_deg = 1
Wall Clock Time per Step --->
Number of Nodes --->