Long-time Simulation of Advection-Diffusion-Reaction System using FEM and FVM on Hybrid CPU/GPU Nodes
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Background
Calcium induced calcium release (CICR) in a heart cell can be modeled by a system of coupled time-dependent advection-diffusion-reaction equations:

\[ u^{(i)}_t - \nabla \cdot (D^{(i)} \nabla u^{(i)}) + \beta^{(i)} \cdot \nabla u^{(i)} = q^{(i)} \]

for the concentrations \( u^{(i)}(x,t) \), \( i = 1, \ldots, n_s \), of the \( n_s \) reactive species

for all points \( x \in \Omega \subseteq \mathbb{R}^d \) (\( d = 1, 2, 3 \)) and time \( 0 < t \leq t_{\text{fin}} \).

The right hand sides \( q^{(i)} \), \( i = 1, \ldots, n_s \), are given by

\[ q^{(i)} = p^{(i)}(u^{(1)}, \ldots, u^{(n_s)}) + s^{(i)}(u^{(1)}, x, t) + f^{(i)}(x, t). \]

- diffusivity matrices \( D^{(i)} \in \mathbb{R}^{d \times d} \), diagonal positive definite
- constant advection vector \( \beta^{(i)} \in \mathbb{R}^d \)
- linear source term \( f^{(i)}(x, t) \) for test problems
- non-linear reaction terms \( p^{(i)} \) couples all PDEs
- application term \( s^{(i)}(u^{(1)}, x, t) \) associated with calcium, \( \lambda^{(i)} = 0 \) for \( i > 1 \)
- Key term \( JSR \) in \( s^{(1)} \) models superposition of CRU injection at all \( x \in \Omega_s \) as point sources:

\[ J_{\text{SR}}(u^{(1)}, x, t) = \sum_{x \in \Omega_s} g S_{\text{SR}}(u^{(1)}, t) \delta(x - \hat{x}) \]

Numerical Methods

Two method of line approaches:

- Spatial discretization using Finite Elements, take advantage of the regular shape of the domain \( \Omega \) and use a uniform mesh of 3-D brick elements.
- Using Finite Volume method, integrate equations over each control volume, using numerical flux functions to approximate diffusive and advective fluxes.

Summary of other numerical methods:

- Time stepping for a large system of stiff ODEs, fully implicit with automatic step size (and order for NDFK) selection: \( 1 \leq k \leq 5 \)
- Non-linear solver: Newton method with analytical Jacobian
- Linear solver: iterative Krylov subspace method family (specifically BiCGSTAB) with matrix-free products for all system matrices and their transposes

\[
\begin{array}{c|c|c|c}
N_x \times N_y \times N_z & \text{DOF} & \text{number of time steps} & \text{memory usage predicted (GB)} \\
\hline
32 \times 32 \times 128 & 421,443 & 58,416 & 0.05 \\
64 \times 64 \times 256 & 3,257,475 & 73,123 & 0.41 \\
128 \times 128 \times 512 & 25,610,499 & 89,088 & 3.24 \\
\end{array}
\]

Simulation of CICR in 3D

Open calcium release units throughout the cell using finite element method. Based on simulation with CUDA + MPI.

CUDA + MPI

The program used to perform the parallel computations presented here is an extension of a C program with MPI for parallel communications. However, to enable efficient calculations on GPU, almost all calculations have been redesigned to take advantage of GPU parallelism.

- Each node has 2 eight-core CPUs, each CPU is connected to a NVIDIA K20 GPU via PCIe bus.
- Minimize data transfer between host and device:
  - Allocate all large arrays on device memory, avoid data transfer in loops
  - Share C struct between host and device
  - Only communicate for output and data exchange between processes
- Reduce time required for MPI communication:
  - Use Non-blocking MPI communication such as MPI_Isend and MPI_Recv, and start MPI command as early as possible
  - Keep GPUs busy while performing MPI communication
- Call MPI_Waitall right before computations involving MPI communicated data

Hybrid Node Schematic

Each node contains two eight-core Intel E5-2650v2 Ivy Bridge CPUs. The 64 GB of the node’s memory are connected to CPUs via 8 memory channels.

The two CPUs of a node are connected to each other by two QPI (quick path interconnect) links.

19 hybrid nodes, each contain two NVIDIA K20 GPUs with 2496 computational cores and 5 GB of global memory.

Nodes connected via quad-data rate (QDR) InfiniBand interconnect.

Storage of more than 750 TB connected by IB.

Results

Wall clock time for FEM on hybrid CPU/GPU in HH:MM:SS and speedup against CPU only runtime on one 16-core node:

Wall clock time for FVM on hybrid CPU/GPU in HH:MM:SS and speedup against CPU only runtime on one 16-core node:

References


Acknowledgments

- HPCF www.umbc.edu/hpcf
- REU Site www.umbc.edu/hpcreu
- CIRC www.umbc.edu/circ
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