**Week 2 update**

Heat Equation Software

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Application Area: FEM

**Summary:**

During the past week, QT interface has been updated with 2D algorithm and default values are provided for the user. All the 2D algorithms are finished. Due to the time limitation, only one 3D algorithm, Backward Euler is implemented. Mpich and OpenMP are used for parallelization.

**Qt update**

Apart from basic Qt features, which include only type-in values, we develop a more advanced interface, which allows the user to choose from available lists of items. Furthermore, based on the input parameters of the previous slot (such as the dimension), the numerical schemes available would be different. A quick example is that for 3-dimensional problem we have only one numerical scheme(Euler method), so once in the dimension slot the 3 is selected, the numerical method slot can only show the Euler method. Another improvement is that if the user doesn’t want to type a lot words in the GUI, there are recommended values available by default for the time step size, spatial step size, total time, number of threads and the output file name. Once the user clicks the button “Submit data”, the parameters that the user specifies will be saved for the computing part in the algorithms in c++ main function, then automatically exit Qt and run c++ main function.



We also add some more function to make the codes more robust for the users. One is that the user can change the input parameters any time before he or she clicks the button “Submit data”.

**2-dimensional and 3-dimensional algorithms update**

Our software project now has been improved to be able to solve the 2-dimensional partial differential heat equation with multiple commonly used algorithms, including Euler, Backward Euler, Crank Nicolson, Dufort Frankel methods and 2D FEM. For explicit schemes (Euler and DuFort Frankel methods), computation has not increase much as no linear system needed to solve. But as for implicit methods (Backward Euler and Crank Nicolson methods), computational consumption has been drastically increased such that it takes around 30 minutes to finish 60x60 points spatial domain in ccv for 10 time steps, in which case the size of the matrix for the linear system to solve reach up to 3600x3600.

The majority of computational effort is used in solving linear equation in explicit methods. The Eigen library has default parallelization set up with OpenMP. So cmake file is modified to enable openmp. Also Mpich is used for multithreads setting in 1D convergence test. With the parallelization setting, a significant decrease in computational time could be obtained.

Based on the previous analysis, for 3-D problem, we have the explicit algorithm Euler method working for the user, which would take a fair amount of time to finish a coarse mesh domain in a few time steps.

Convergence and stability testing for 2D was added to the program. The functions evaluate behavior for long time to check for convergence.

Visualization was extended to the output of the 2D algorithms. The output printing function was modified to format the output data in order to be processed by gnuplot. The gnuplot script plots each time step and combines each plot to produce an animated picture format video over the time steps. The script also produces animations for all data files within the directory without needed to be called repeatedly. The 2D plots are heat maps of the data values, which makes it easy to visualize the change over time of the function. The animations do not open automatically because they can be large files, so the user needs to select the files for viewing.

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| Major tasks accomplished | Description |
| whole project | Finish all the 2D algorithms. Add new features to QT interface. Use bash script to link QT, main function, and visualization. Enable openmpi and openmp for multithreads. Add 2D visualization features. |
| Zhi Li | 2D FEM algorithm. 3D Backward Euler method. Multithreads for convergence algorithm. Bash script to link separate parts. |
| Helena Liu | Extend visualization module to 2D version. Convergence and stability test for 2D version. |
| Yunxing SU | Update new Qt features. Write 2D version for Euler, DuFort Frankel, Backward Euler and Crank Nicolson algorithms. |