ENGINEERING AT ILLINOIS

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Analyzing the Scalability of Nek5000

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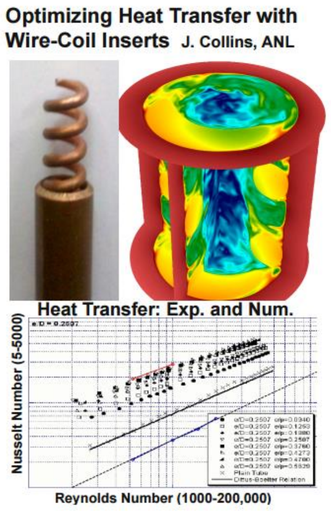
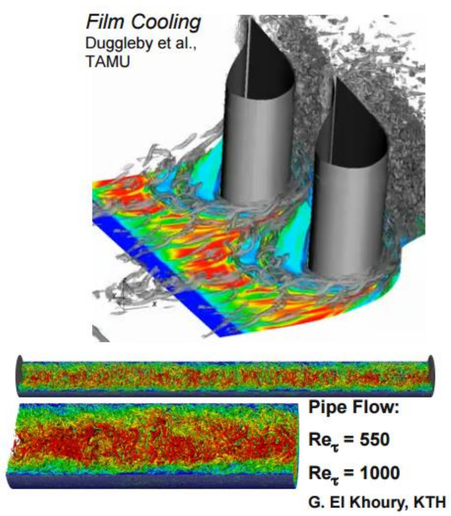
Computational Fluid Dynamics (CFD)

- The study of fluids that solves fluid flow problems algorithmically and with numerical analysis techniques
- Simulates the interaction of liquids with the surfaces around them, defined by "boundary conditions"
- Applicable to domains such as heat transfer, particle tracking, and free surface flow

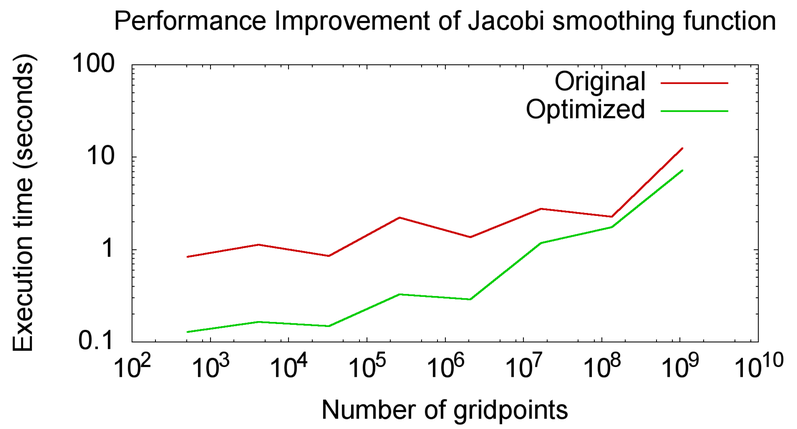




Goal & Early Research

- Overall goal: analyze and push the scalability of Nek5000 on 1000's of processors, identifying bottlenecks that are preventing further scaling (is it communication- or computation-bound?)
- Had to learn Fortran77 from scratch beginning with some multigrid code (similar to what is found in Nek5000) called x2p.f
- Then had to learn the Blue Waters execution environment, starting with x2p but then moving on to Nek5000 itself
- Nek5000's "timing" example case (containing ping-pong and all_reduce tests) was used to re-establish benchmarks for communication time on Blue Waters
- Researched into potential programming optimizations using modern MPI features - e.g. MPI Datatypes, Shared Memory Access
- Investigated various profiling tools that might be used to identify the bottlenecks

Other Results

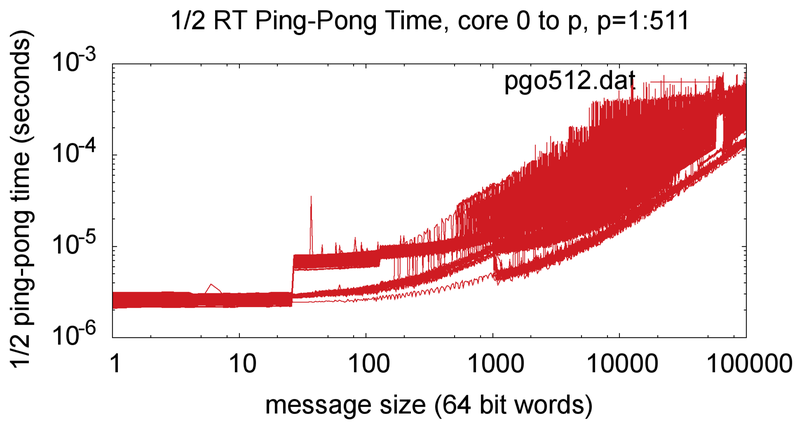


- Had some success with using MPI Datatypes and variable switching to speed up the multigrid code mentioned under "Goals"
- Developed script to automatically run ping-pong test, then parse the descriptive logfile output and graph the data
- Created a series of scripts to consolidate Nek5000 configuration in one config file
- Fixed parameters and restrictions preventing ping-pong from running on 32768 processors

Nek5000

- Very extensive CFD library capable of most/all math required by a simulation
- ~125k lines of Fortran77, and ~18k of C, with MPI support for massive parallelization
- Used by Argonne National Laboratory
- Demonstrates good parallel speedup and strong scaling to one million MPI ranks
- As the Wiki says, the weakest part of Nek5000 is by far the documentation…

Ping-Pong Test



Further Work

- More profiling needs to be done on typical use cases to identify the bottlenecks
- The Blue Waters compilation flags should be experimented with to determine the best acceptable flags for Nek5000
- More easily accessible documentation!

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