Performance of FORTRAN and C GPU Extensions for a Benchmark Suite of Fourier Pseudospectral Algorithms

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Abstract

A comparison of PGI FORTRAN CUDA, Nvidia CUDA and PGI OpenACC implementations of pseudospectral methods on a single GPU and GCC FORTRAN on single and multiple CPU cores is reported. The GPU implementations use CuFFT and the CPU implementations use FFTW. Porting pre-existing FORTRAN codes to utilize GPUs is efficient and easy with OpenACC or FORTRAN CUDA.

Equations

Cubic Nonlinear Schrödinger

$$iu_t + u_{xx} + u_{yy} = |u|^2 u$$

This equation arises in a variety of contexts including quantum mechanics, in simplified models for lasers, and water waves. The numerical solution is obtained using a splitting method where the linear part is solved in Fourier space and the nonlinear part in real space [2].

Sine-Gordon Equation

$$u_{tt} - \Delta u = -\sin u$$

This equation arises in many different applications, including propagation of magnetic flux on Josephson junctions, and sound propagation in a crystal lattice. The time derivative is approximated by a central difference.

2D Navier-Stokes Equation

$$\Delta\omega = \mathrm{Re}\,(\omega_t + \psi_y\omega_x - \psi_x\omega_y)$$
$$\Delta\psi = -\omega.$$

Time is discretized using the Crank-Nicolson method, where the nonlinear terms are solved using fixed point iteration. ψ is the vorticity, ω the streamfunction and Re is the Reynolds number.

All equations are solved spatially using Fourier pseudospectral methods and all nonlinear terms are solved in real space.

Example Simulations

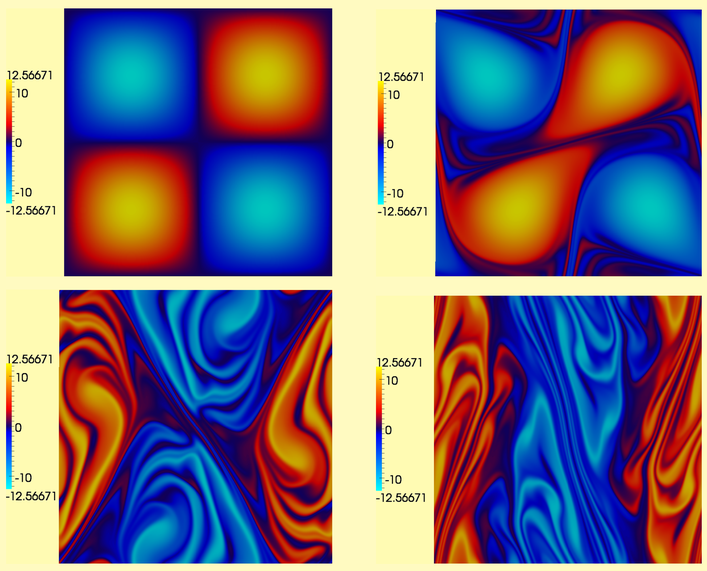

Figure 1: Vorticity evolution of a small perturbation to the Taylor-Green vortex solution to the Navier-Stokes equation at $Re = 6 \times 10^4$ on a $[0,1]^2$ domain. Plots are at times = 0, 5, 8, and 9. The timestep was approximately 10^{-5} and resolution was 1024^2. The images show initial breakup of the vortex, the ensuing turbulence and then decay to zero.

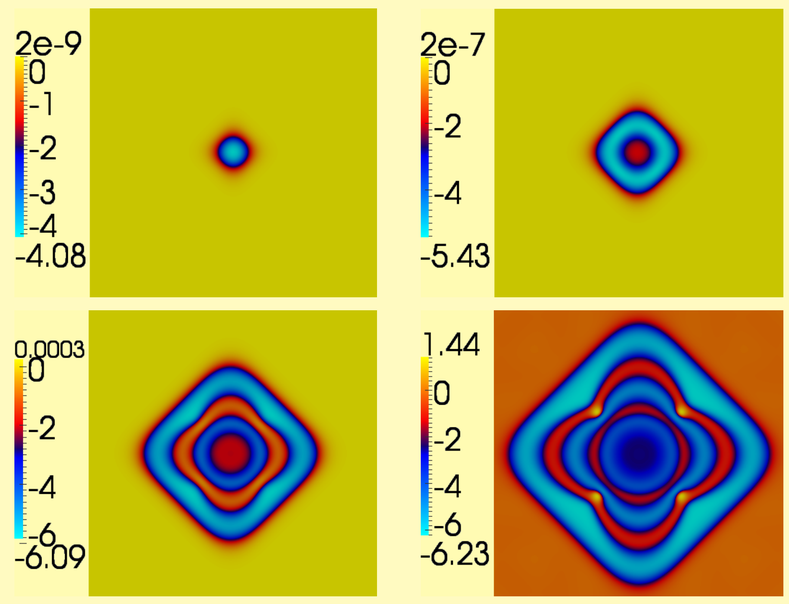

Figure 2: A stationary breather solution to the sine-Gordon equation from [1]. The timestep was 2.5×10^{-4} on a domain $[-40\pi, 40\pi]^2$ with $u(t=0) = -4\mathrm{atan}\,[0.044\mathrm{sech}(0.4x)\mathrm{sech}(0.4y)]$ and $u_t(t=0) = 0$.The solution is seen to oscillate in place while slowly expanding.

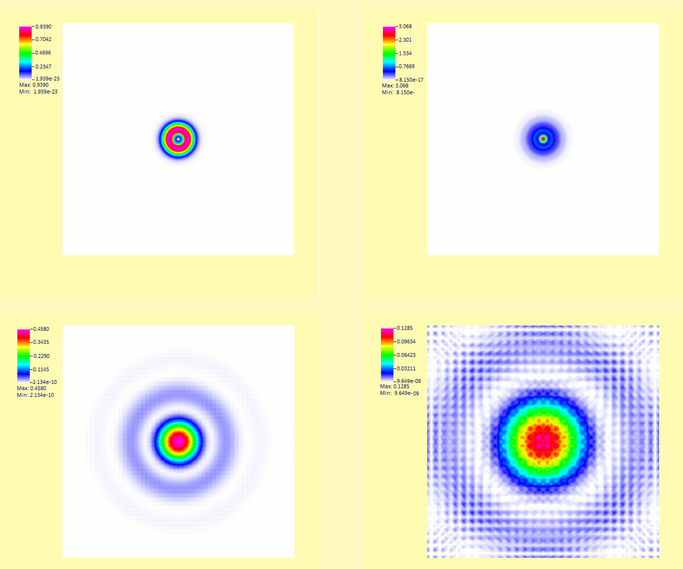

Figure 3: Plots of $|u|^2$ for the cubic nonlinear Schrödinger equation on a $[-3\pi, 3\pi]^2$ domain at $t = 0.05, 0.1, 0.5$ and 1.0. The initial condition was $1.1(1 + 5(x^2 + y^2 - 1))^{-1}$. The timestep was 10^{-4} and resolution was 2048^2. The solution focuses, then disperses and finally interacts with itself since it is on a periodic domain.

Benchmark Results

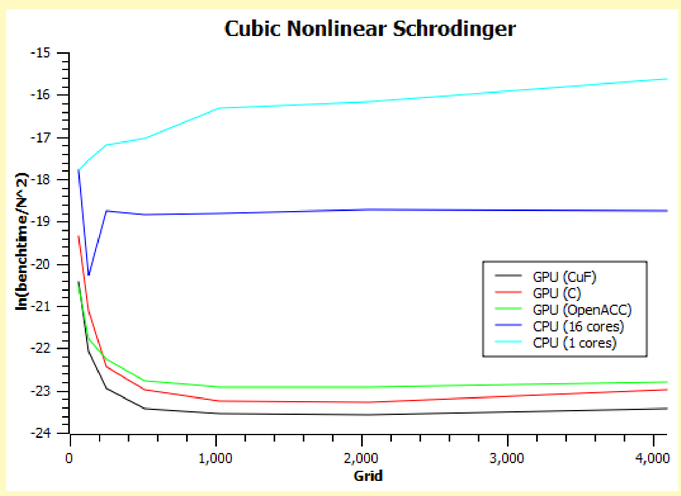

Figure 4: Computation times in seconds for 20 time steps of $\delta t = 10^{-5}$ for the Cubic Nonlinear Schrödinger equation on $[-5\pi, 5\pi]^2$

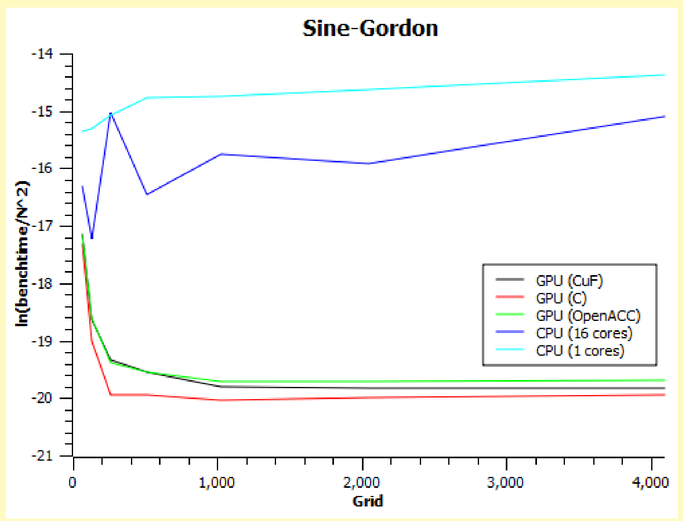

Figure 5: Computation times in seconds for 500 time step of $\delta t = 10^{-3}$ the Sine-Gordon equation on $[-5\pi, 5\pi]^2$.

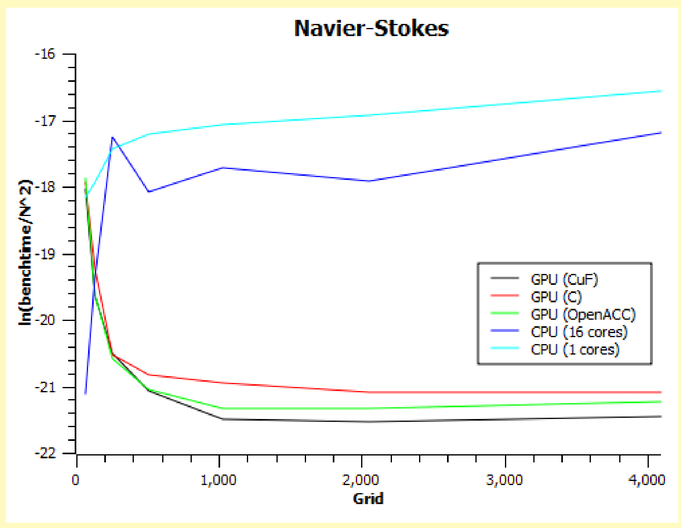

Figure 6: Computation times in seconds for 20 time steps of $\delta t = 1.25 \times 10^{-3}$ for incompressible Navier-Stokes equation on $[0,1]^2$.

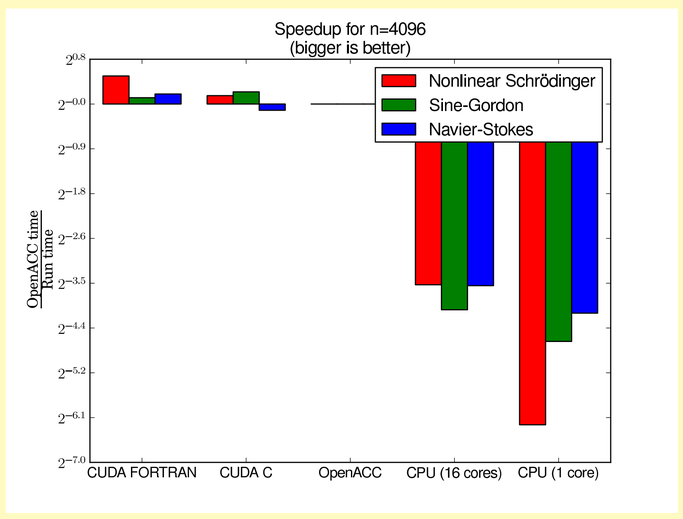

Figure 7: Speedup for GPU and CPU runs.

Conclusion

GPUs provided significant but differing performance improvements for all our codes compared to CPUs. CUDA FORTRAN and OpenACC provide several directives that make programming simpler than CUDA C.

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References

[1] Minzoni, AA, et. al. "Evolution of two-dimensional standing and travelling breather solutions for the Sine–Gordon equation", Physica D 189, 2004.

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