How We Crammed a Black Hole, a Star Cluster, & a Turbulent Plasma into a GPU (and lived to talk about it)

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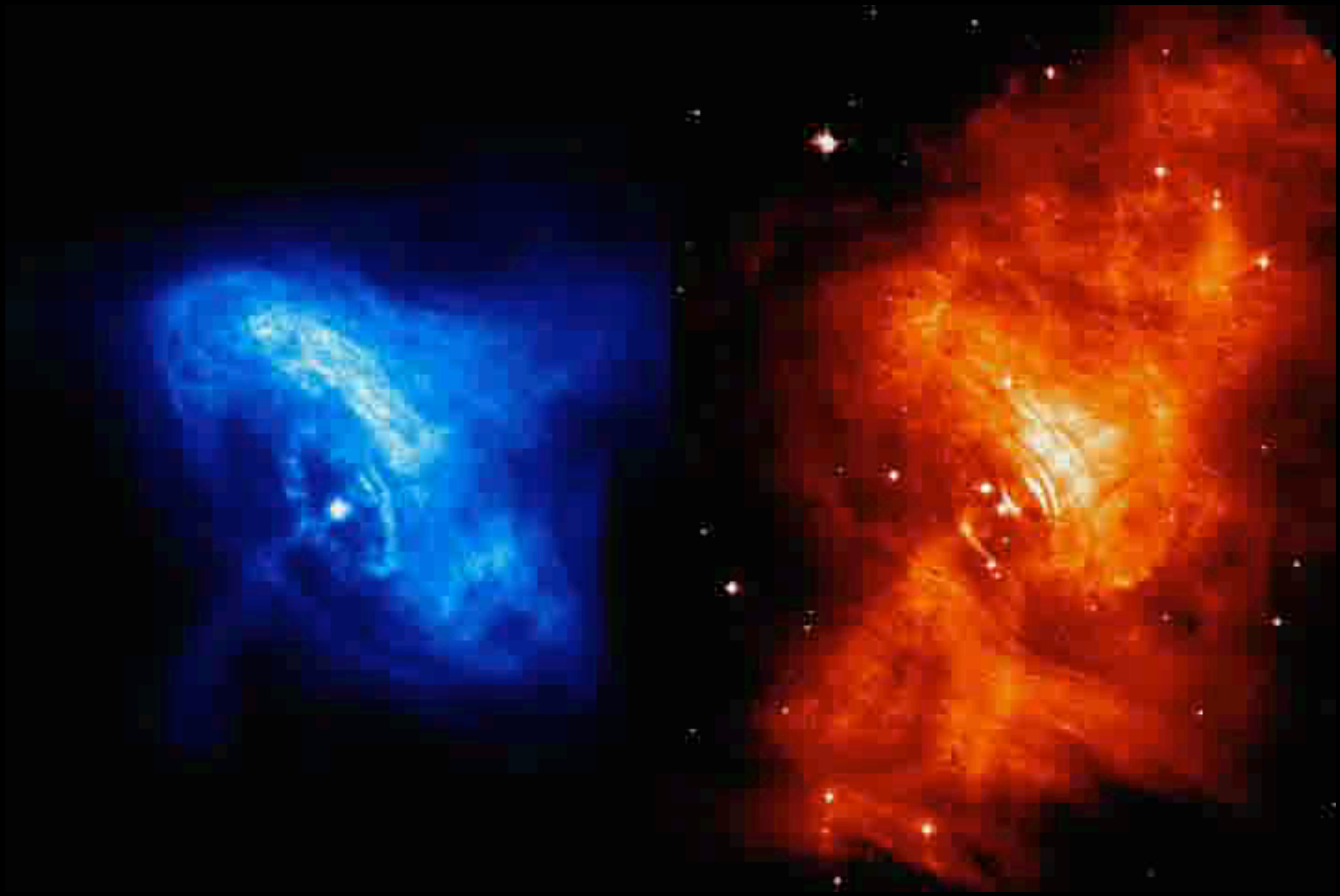
Advanced Viz: A Black Hole

Milky Way in X-Rays from Chandra

Pulsar in Crab Nebula: Chandra, Hubble



Everything you can see in these pictures is associated with super-hot, turbulent plasma (ionized gas).

To understand the details, one needs to understand how astrophysical objects turn gravitational energy into light.

This requires high-performance computing, now being accelerated with NVidia GPU's.

Moore's Law ++

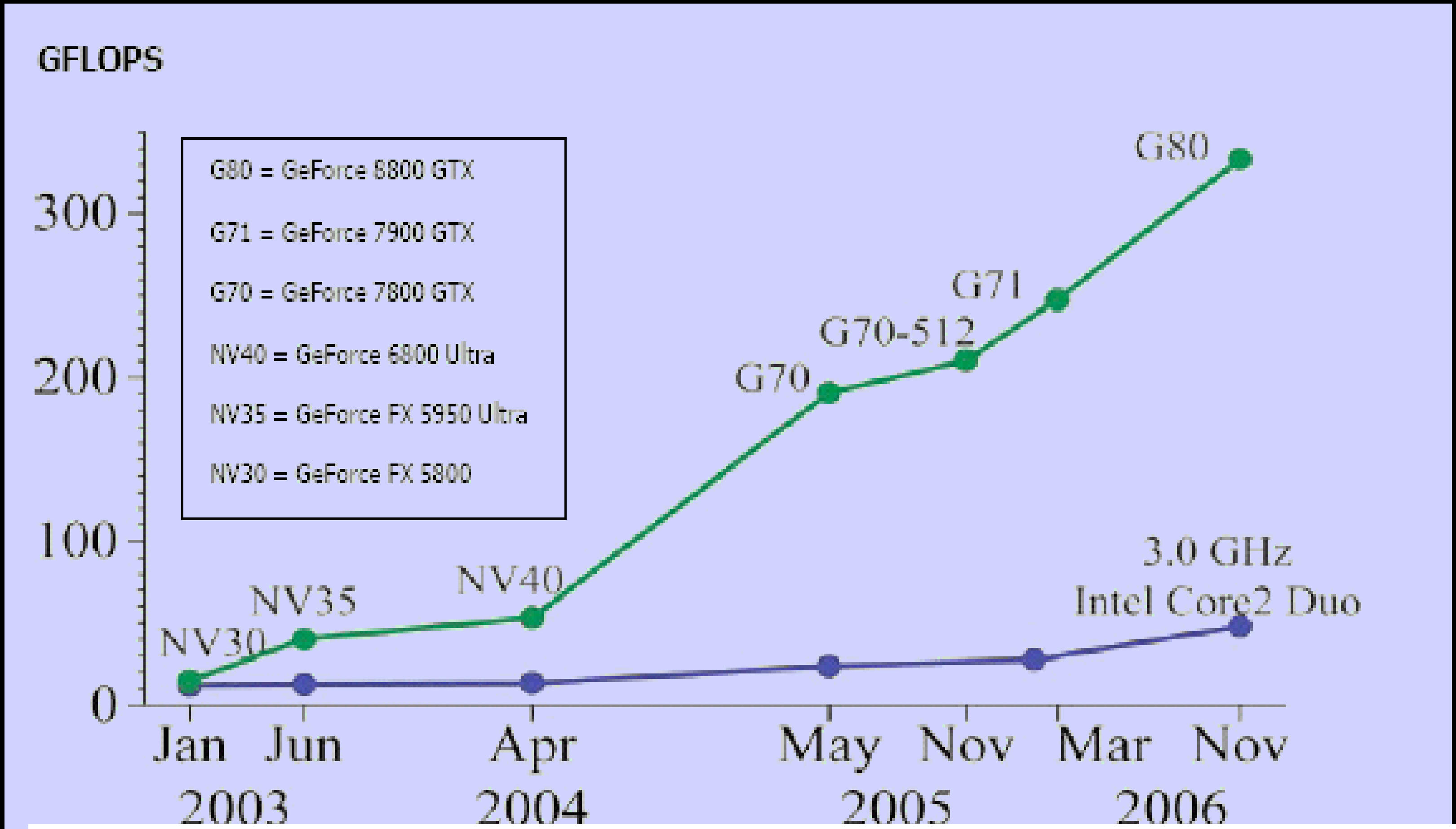
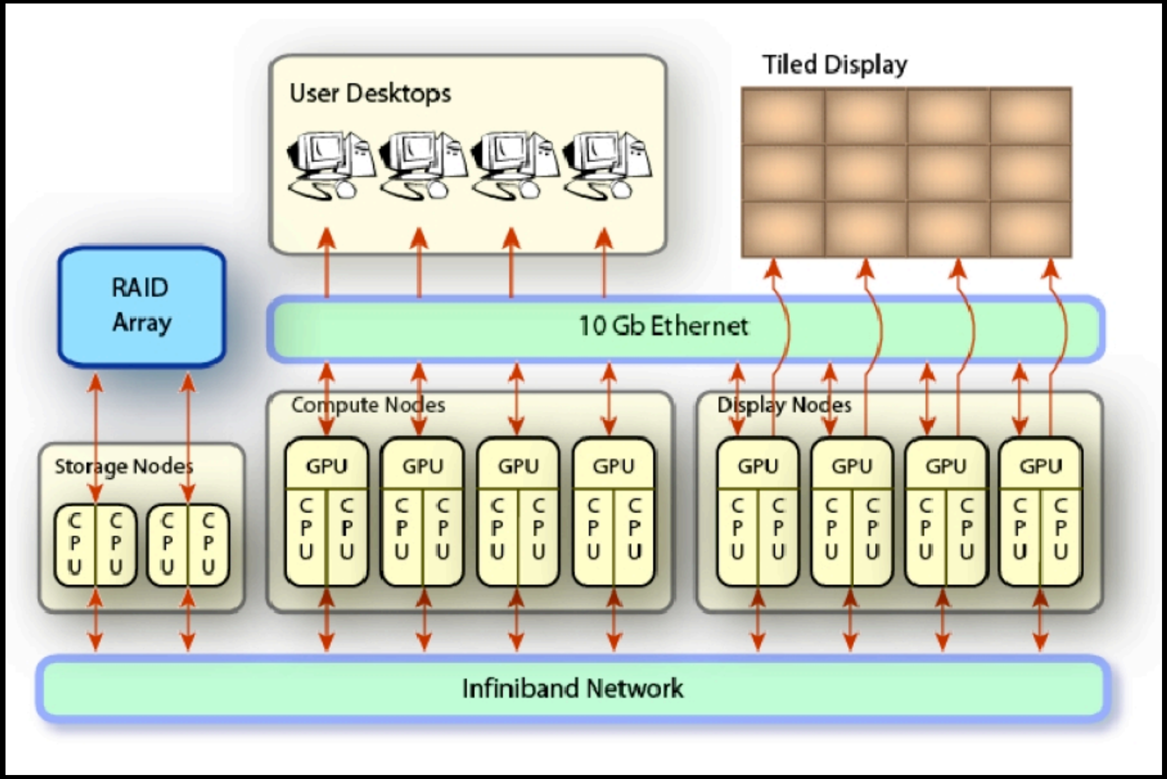


Fig. 1 Relative gigaflop ratings of state of the art Intel CPUs and NVIDIA GPUs

Overview

- Maryland effort: who, what, why
- Working physics algorithms
  1. FMM (N-body, other uses)
  2. Pseudo-spectral turbulence
  3. Particle-in-cell turbulence
  4. Also audio and visual computing on GPU's, optimization, large-scale visualization algorithms, etc
- Results of integration: Middleware library to accelerate development in Fortran 9x: ***Flagon***
- Maryland roadmap

Maryland GP-GPU hardware



NSF-funded CPU/GPU cluster with:

15 display nodes

12 computer nodes

3 storage nodes

1 console node

1 scheduler node

10 TB storage

CPUs: 3 GHz Xeon

GPUs: various nVidia models

Upgrade scheduled

Who is involved at UM?

- Effort began in UMIACS (UM Inst for Advanced Comp Studies)
- Focus broadened to include physics, astrophysics
- Weekly meetings of 5-20 with discussions, informal talks
- Undergraduates, graduate students and post-docs from outside UMIACS now more deeply involved.
- Funded research in GPU's from NSF, DOE, NASA, DARPA
- Current astrophysics-GPU projects: Turbulent heating, MHD turbulence, Numerical relativity

Key Questions Addressed

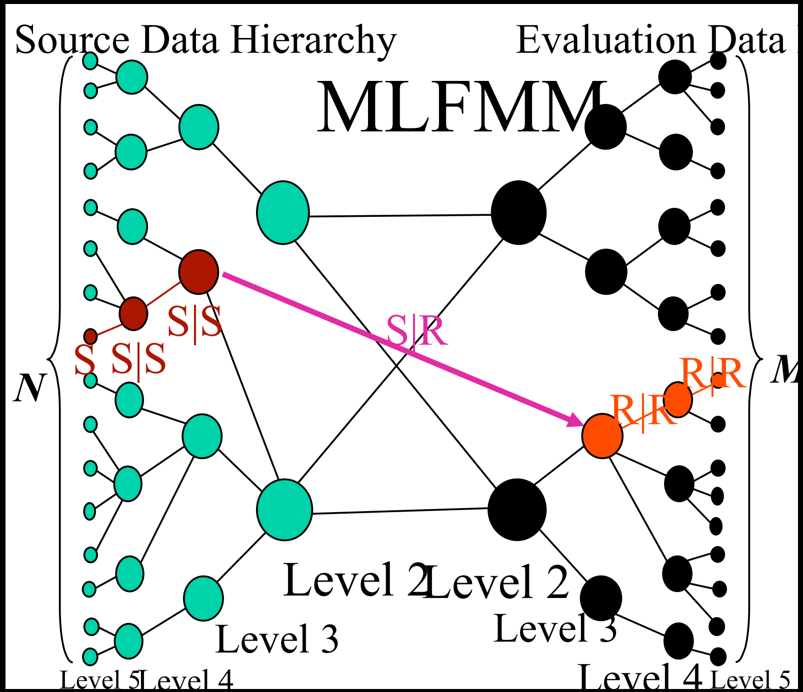
- How stable is the hardware + software platform?
- Which major algorithms can successfully exploit GPU hardware?
- What is the development and maintenance path for porting large-scale applications to this platform? Is there a net benefit? Or is the programming model too cumbersome?
- Which algorithms can exploit clusters of GPU's?
- Aiming for a $1-5M purchase in 2008-09 timeframe. CPU? GPU? Which vendor?

Refuting the Moore's law argument

- Argument ~ Wait for processor speed to solve complex problems, without algorithm improvement
- Is this true?
- Yes, for algorithms with linear asymptotic complexity
- No!! For algorithms with different aymptotic complexity
- Most scientific algorithms ~ N^2 or N^3
- For a million variales, we would need about 16 generations of Moore's law before an N^2 algorithm was comparable with an *O(N)* algorithm.
- Implies need for sophisticated algorithms, but are they programmable on a GPU?

Fast Multipole Methods

- Follows from seminal work of Rokhlin and Greengard (1987)
- General method for accelerating large classes of dense matrix vector products
- Reduce computational/memory complexity from O(N*N) to O(N)
- Allow reduction of O(N*N) and O(N*N*N) operations to linear order
- Involves intricate programming with sophisticated data structures
- Recursive tree transverses



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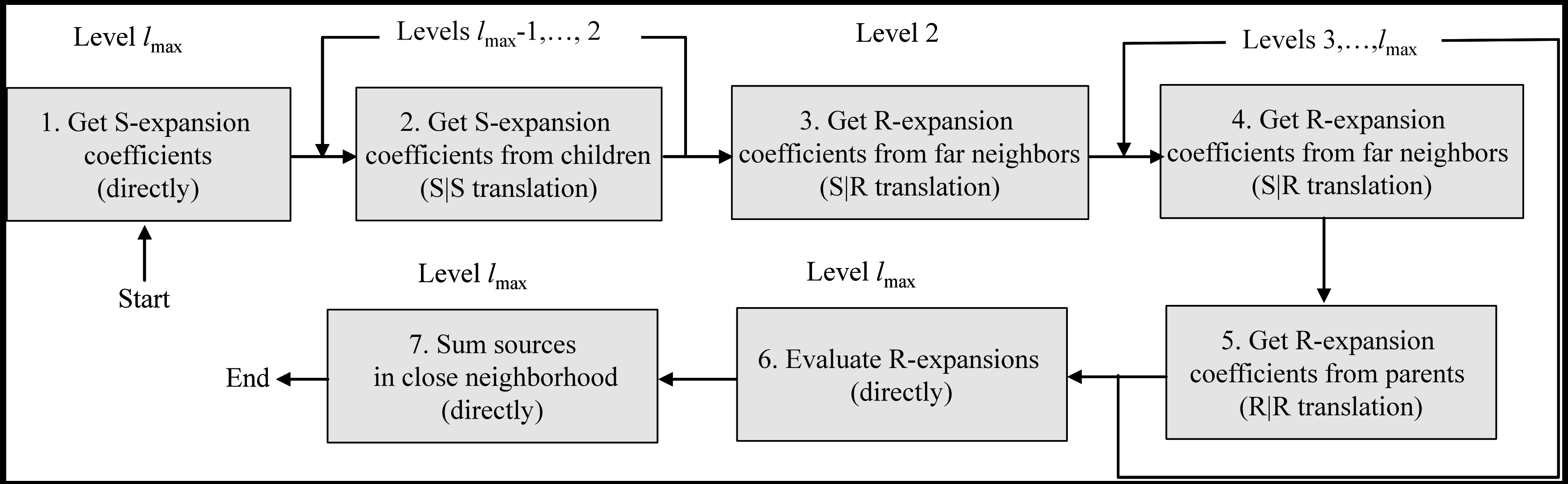


Challenges

- Complex FMM data structure
- No simply mapping to SPMD architecture
  - non-uniformity of data causes problems with efficient work load (taking into account large number of threads)
  - serial algorithms use recursive computations
  - existing libraries (CUBLAS) and middleware approach only get us part of the way
  - high performing FMM functions should be redesigned and written in CU
- Low amount of fast (shared/constant) local memory for efficient implementation of translation
- Absence of good debugging tools for GPU

Performance

N=1,048,576 (potential only)

	serial CPU	GPU	Ratio
p=4	22.25 s	0.683 s	33
p=8	51.17 s	0.908 s	56
p=12	66.56 s	1.395 s	48

N=1,048,576 (potential+forces (gradient))

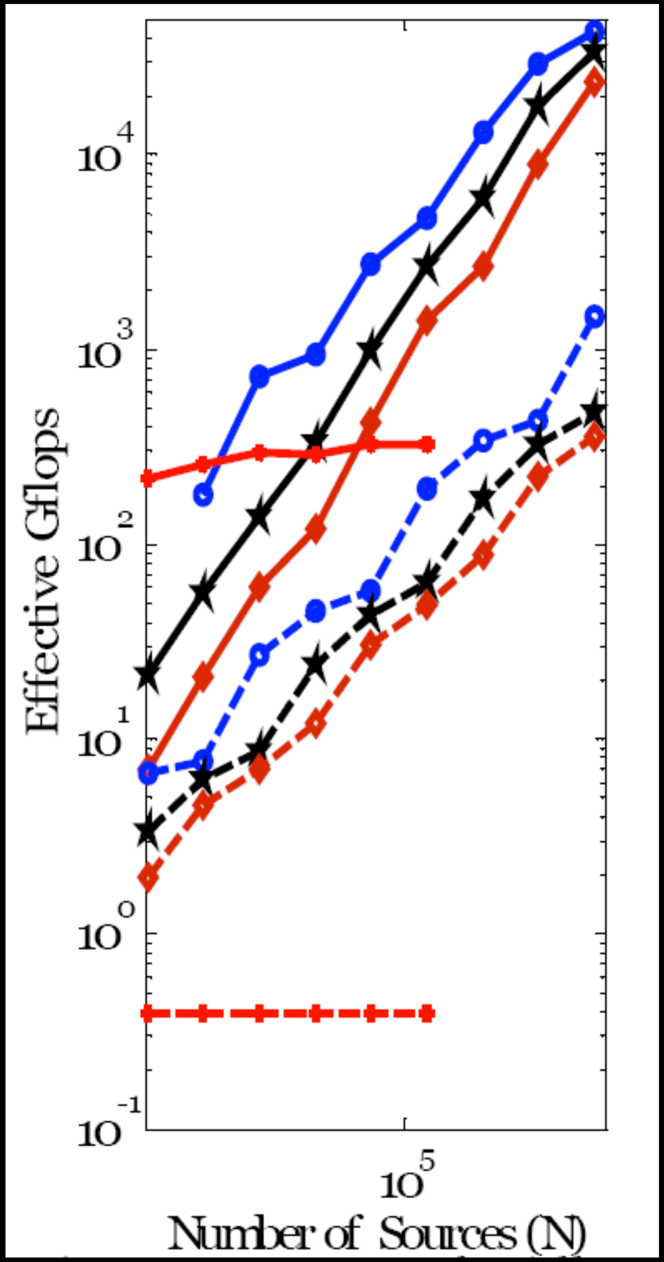
	serial CPU	GPU	Ratio
p=4	28.37 s	0.979 s	29
p=8	88.09 s	1.227 s	72
p=12	116.1 s	1.761 s	66

Performance

Computations of the potential and forces:

Peak performance of GPU for direct summation 290 Gigaflops, while for the FMM on GPU effective rates in range 25-50 Teraflops are observed (following the citation below).

M.S. Warren, J.K. Salmon, D.J. Becker, M.P. Goda, T. Sterling & G.S. Winckelmans. “Pentium Pro inside: I. a treecode at 430 Gigaflops on ASCI Red,” Bell price winning paper at SC’97, 1997.

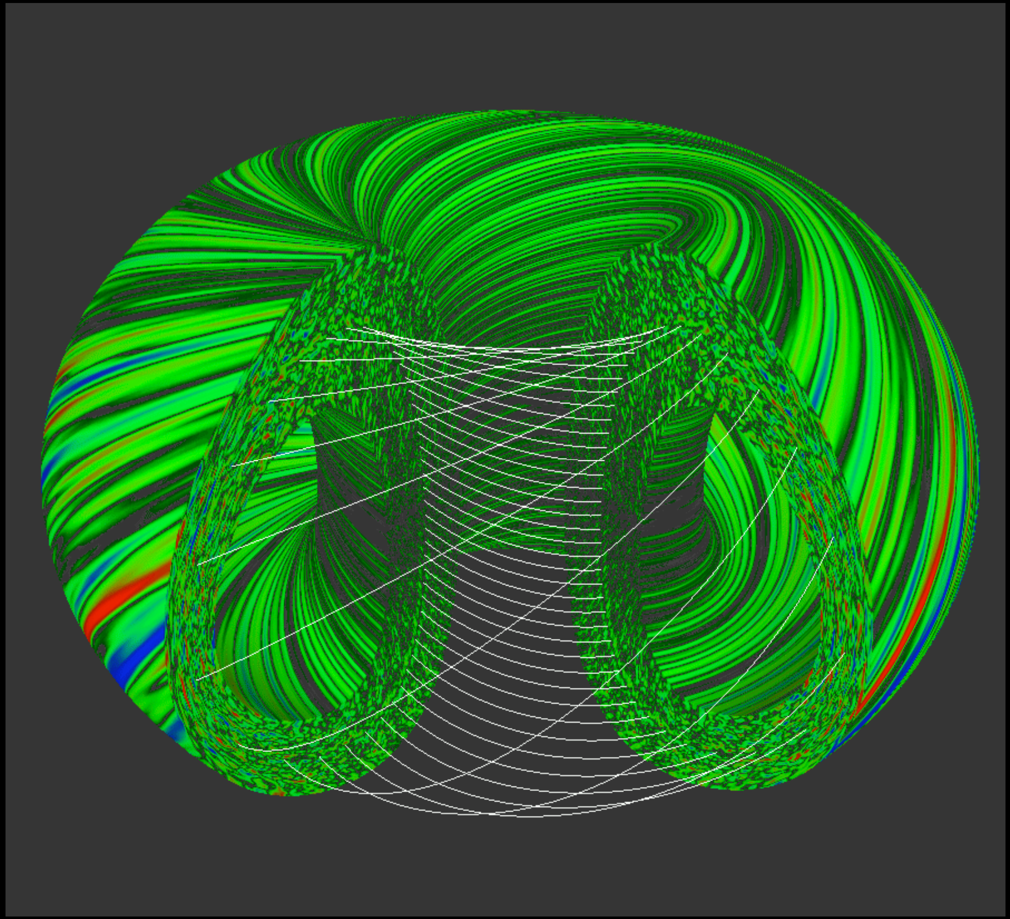


First conclusion: GPU can handle sophisticated algorithms

really well!

Turbulence theory is guided by computation/simulation

- Properties of plasma turbulence are important in laboratory experiments (such as fusion research), in space physics (solar wind), and in astrophysics (ISM, accretion flow luminosity)
- Most computations from Maryland carried out at national supercomputing facilities, on hundreds to thousands of processors.



Fusion turbulence

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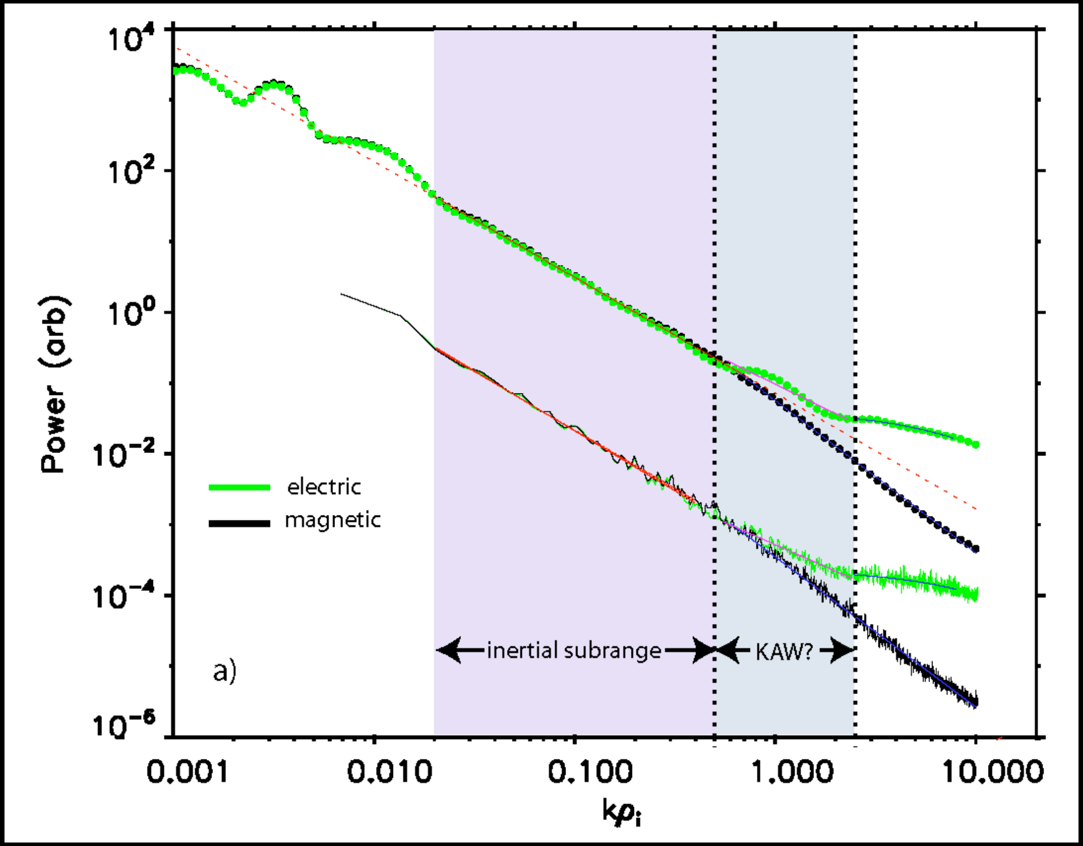

Solar wind turbulence *[Bale, et al, 2005]*

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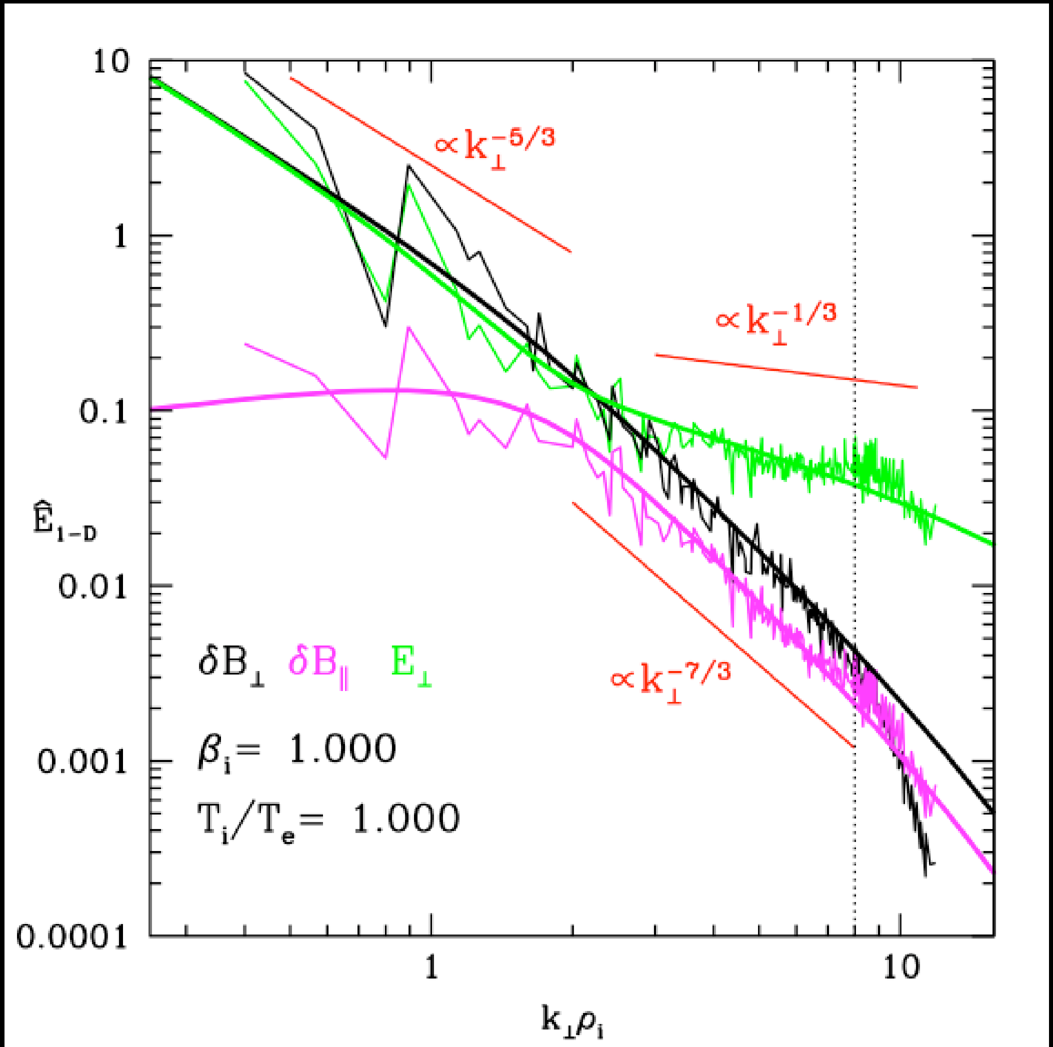

First-principles simulations *[Howes, et al, 2007]*

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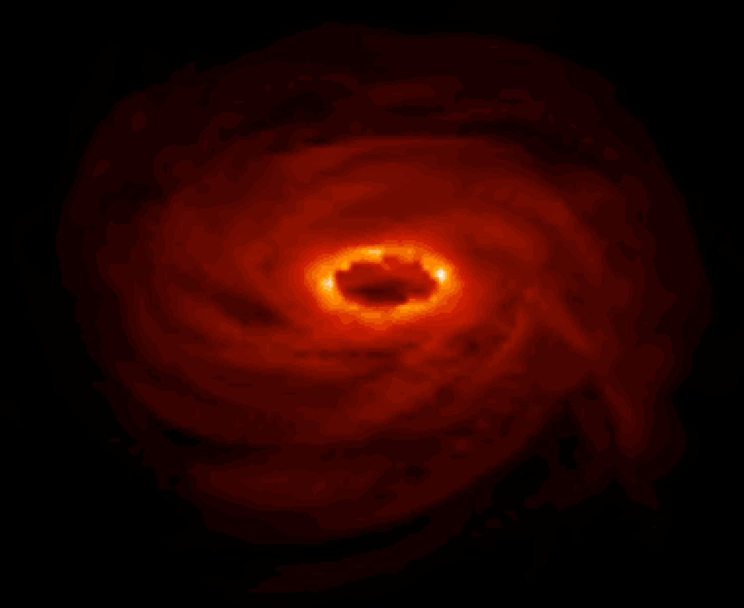

Accretion flow luminosity
[Goldston, Quataert, Igumenshchev, 2005]

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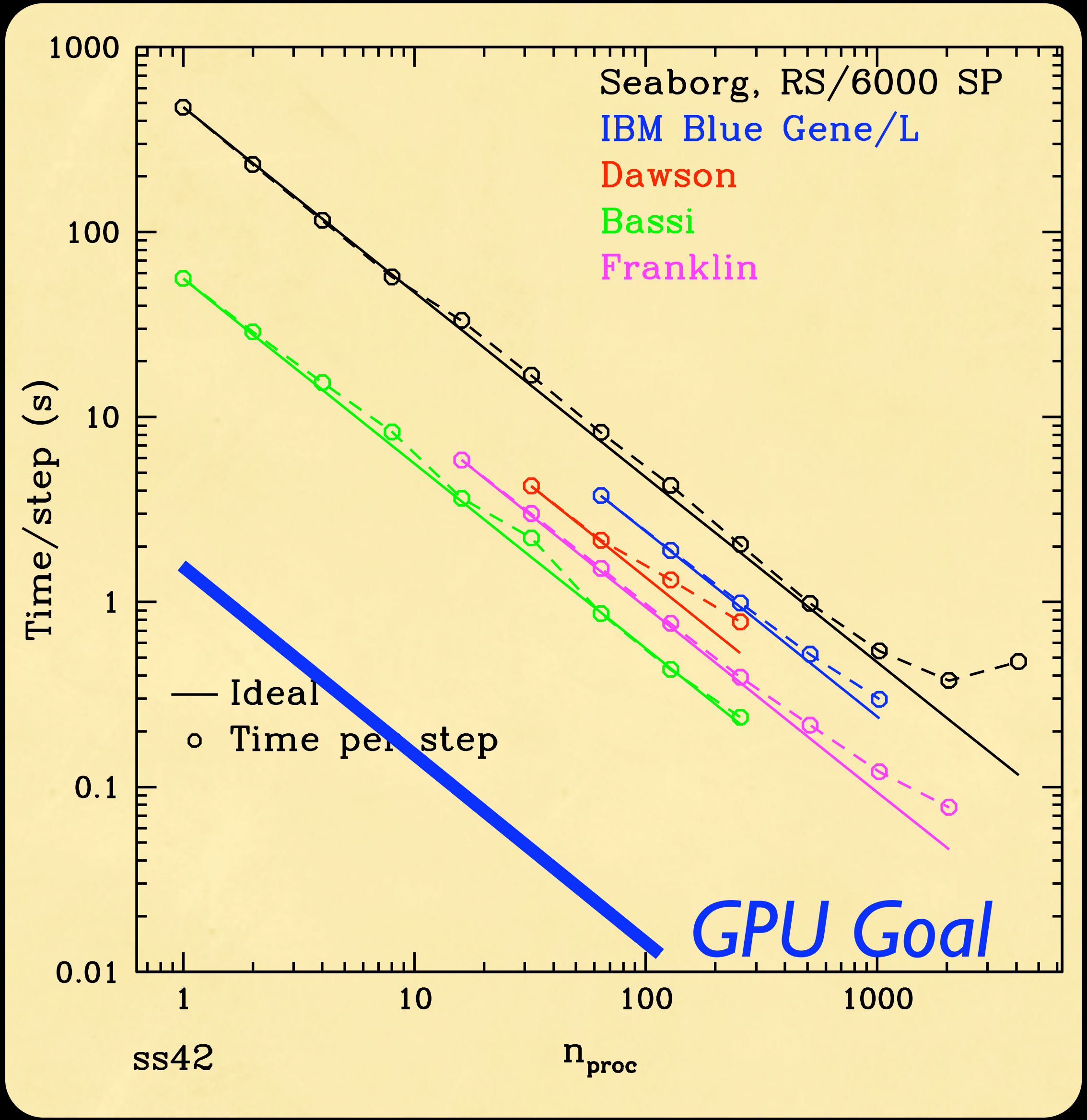
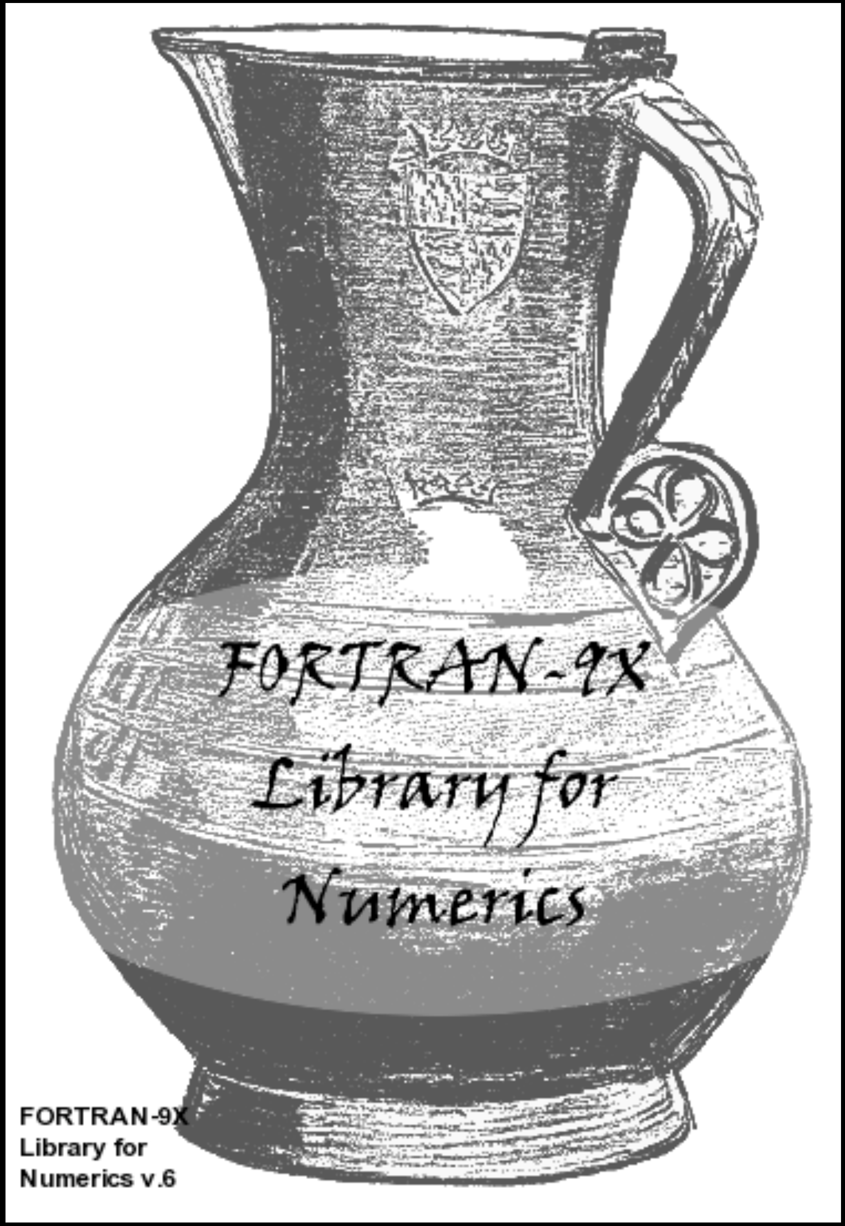


Conversion of legacy Fortran 9x code important to scientific community

- Maintainability, portability
- Developed **Flagon**, an F9x wrapper to ease transition to CUDA
- Flagon available at Sourceforge as Open Source project



Conversion of legacy Fortran 9x code important to scientific community

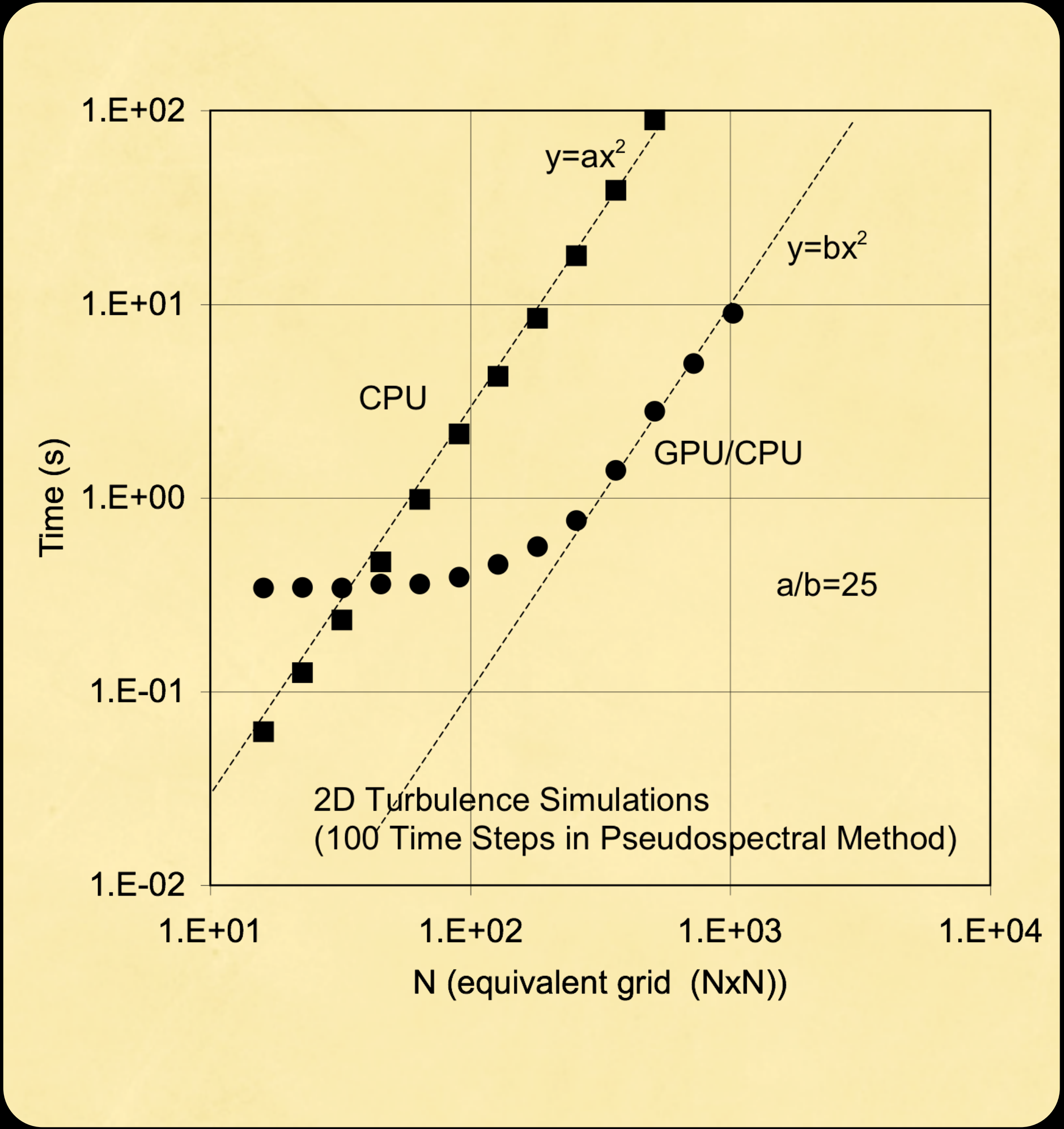
Original Fortran Code

```
subroutine nlterms(isave,a,b,nl)

use com_module


complex,dimension(:,:),intent(in)  ::a,b
complex,dimension(:,:),intent(out)::  nl
integer ::  isave

if(isave /= 1) then
     kxa2=ikx*a
     kya2=iky*a
     call fftwnd_f77_one(plan_f,kxa2,kxa2)
     call fftwnd_f77_one(plan_f,kya2,kya2)
endif

if(isave /= 2) then
     kxb2=ikx*b
     kyb2=iky*b
     call fftwnd_f77_one(plan_f,kxb2,kxb2)
     call fftwnd_f77_one(plan_f,kyb2,kyb2)
end if

nl=kxa2*kyb2-kxb2*kya2
call fftwnd_f77_one(plan_b,nl,nl)
nl=nl*scale

end subroutine nlterms
```

Modified Fortran Code

```
subroutine dev_nlterms(isave,dv_a,dv_b,dv_nl)

use dv_com_module
use mod_devObject

type(devVar),intent(in)  ::  dv_a,dv_b
type(devVar),intent(out)::  dv_nl
integer ::  isave

if(isave /= 1) then
     call devf_mul1(dv_kxa2,dv_kya2,dv_ikx,dv_iky,a)
     call devf_fft(dv_kxa2,fftplan)
     call devf_fft(dv_kya2,fftplan)
endif


if(isave /= 2) then
     call devf_mul1(dv_kxb2,dv_kyb2,dv_ikx,dv_iky,b)
     call devf_fft(dv_kxb2,fftplan)
     call devf_fft(dv_kyb2,fftplan)
endif


call devf_mul2(dv_nl,dv_kxa2,dv_kyb2,dv_kya2,dv_kxb2)
call devf_ifft(dv_nl,fftplan)
call devf_mul(dv_nl,dv_nl,dv_scale)

end subroutine dv_nlterms
```

GPU Performance Achievable by Non-Expert



Plasma turbulence code (Orzag-Tang problem) ported from existing Fortran 95 code in one day achieves 25x speedup

GPU non-expert (me)

Expert (Despain) then upped to 32x

Second conclusion: GPU can handle Fortran 9x and spectral/global algorithms

really well!

Summary of Performance Results

- MHD: 25x speed-up (nonlinear PDE's) -- recently upped to 32x (Despain)
  - FFT's, data-parallel. Very easy to exploit
- N-body force calculation with FMM on GPU: 1M masses in 1 second
  - Memory hierarchy, custom algorithm. Successfully exploited.
- Particle-in-cell: 7-20x speedup.
  - Need coalesced writes to get best performance; without sorting, can achieve ~ 100x speedup, but sorting is required to avoid memory bottleneck

Key early finding: Needed another layer to support easy porting, debugging and maintenance of Fortran 9x legacy codes. Developed Flagon. Happy to talk more about this at Astrophysics Roundtable, tomorrow AM.

Roadmap

- Now working on numerical relativity (with M Tiglio and M Mahmud)
- Upgrading current cluster
- Major questions remaining to be answered:

1. Multi-GPU computing necessary for astro apps we care about
    - Current and continuing focus
2. Other vendors may "win" -- don't want to be stuck with a Connection Machine...
    - Cell BE, AMD/ATI, Larrabee
3. Is development platform rich enough for GPU non-experts?