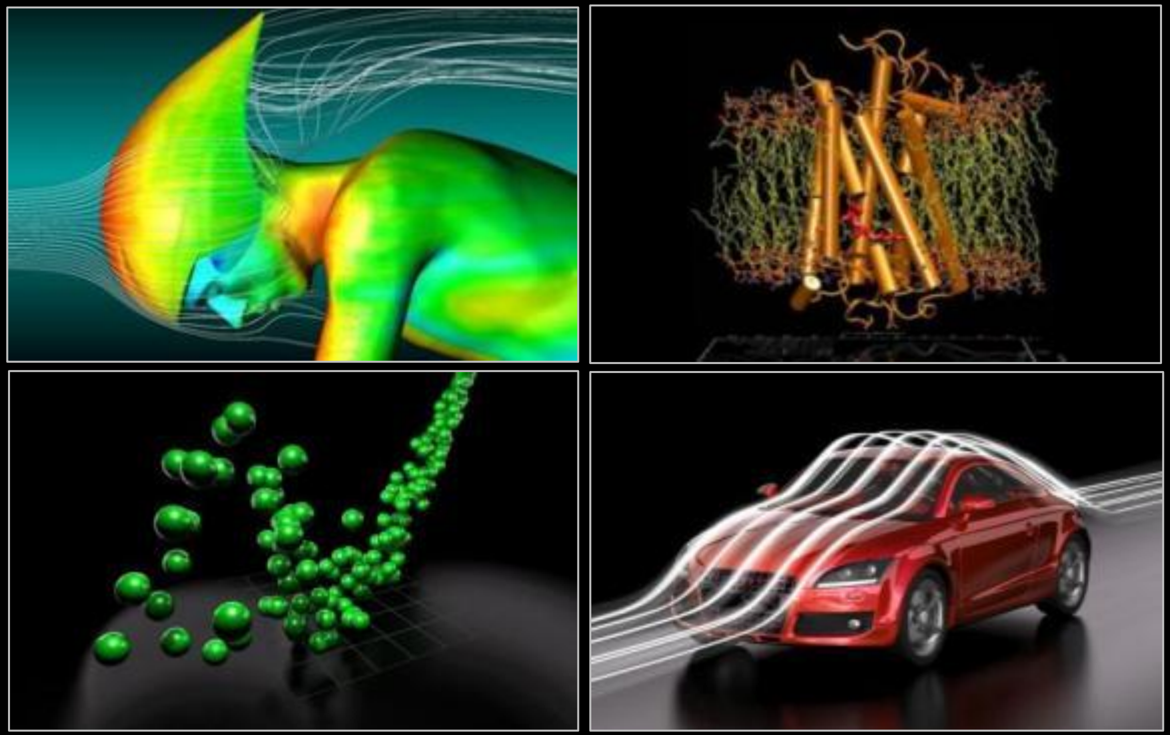


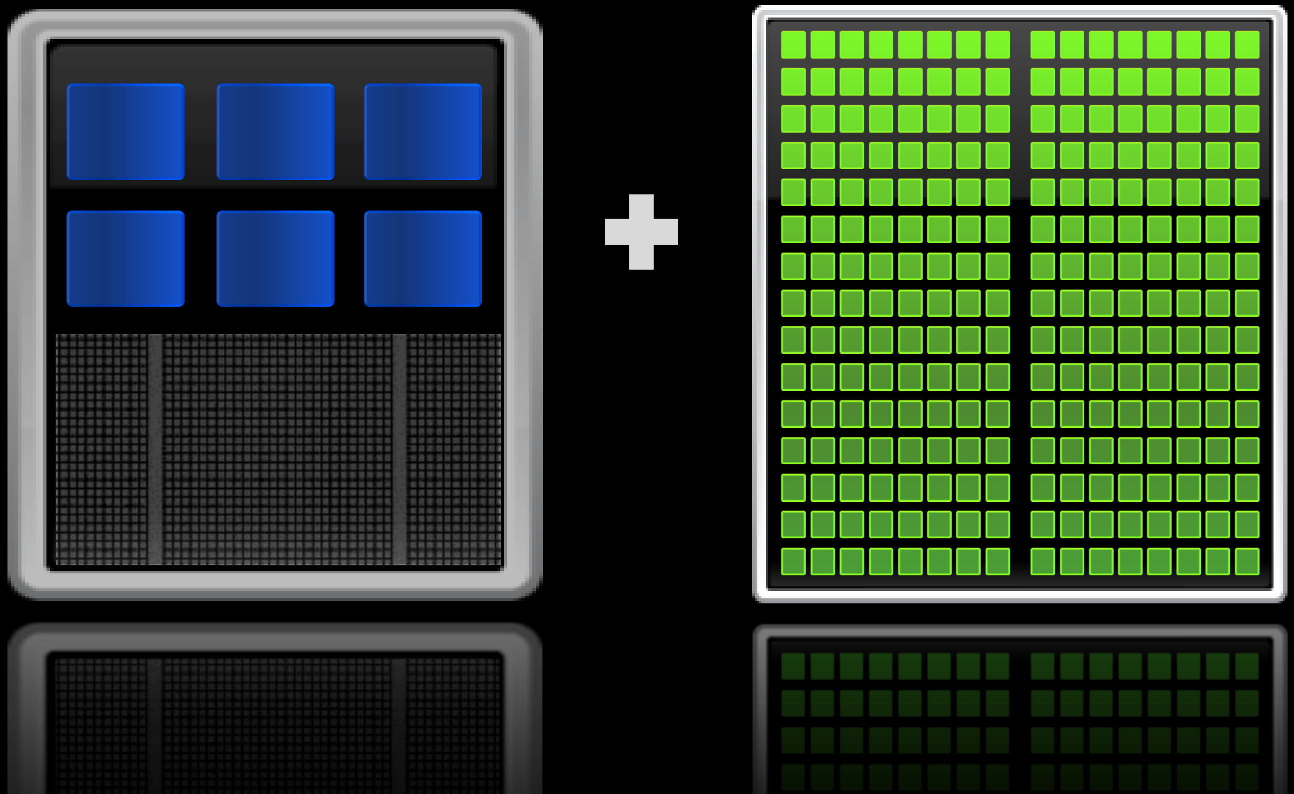
GPU Programming with CUDA and OpenACC

Axel Koehler - NVIDIA

Heterogeneous Computing

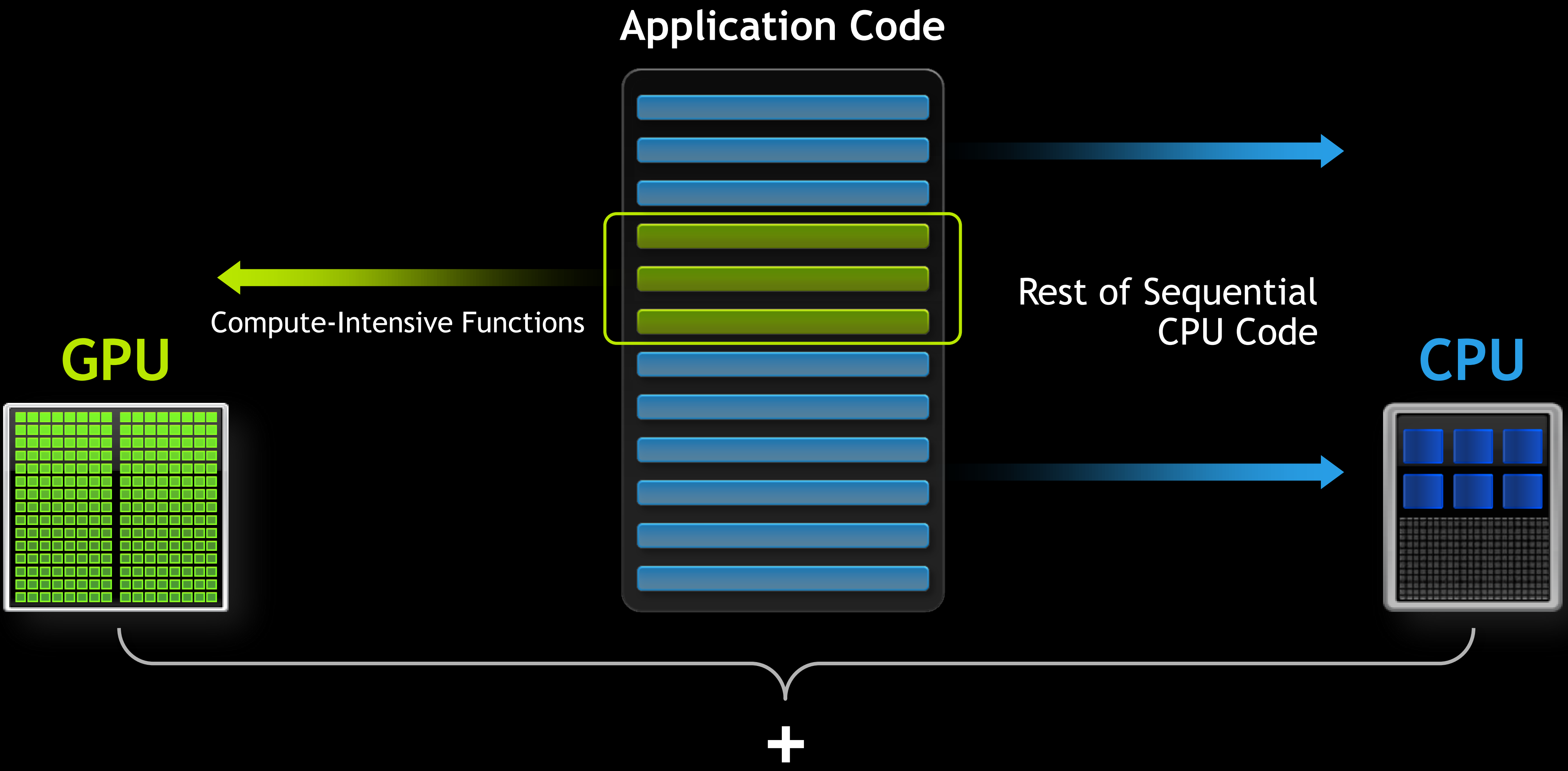
Add GPUs: Accelerate Applications

CPUs: designed to run a few tasks quickly.



GPUs: designed to run many tasks *efficiently*.

Minimum Change, Big Speed-up



Ways to Accelerate Applications

Applications

Libraries

Directives

Programming Languages (CUDA, ..)

High Level Languages (Matlab, ..)

Easiest Approach

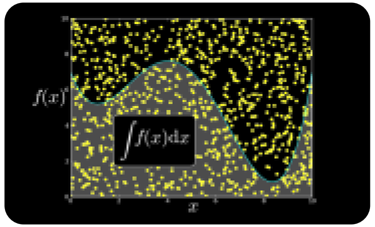
Maximum Performance

No Need for Programming Expertise

GPU Accelerated Libraries

“Drop-in” Acceleration for Your Applications

NVIDIA cuBLAS



NVIDIA cuRAND

NVIDIA cuSPARSE

NVIDIA NPP

Vector Signal Image Processing

GPU Accelerated Linear Algebra

Matrix Algebra on GPU and Multicore

NVIDIA cuFFT

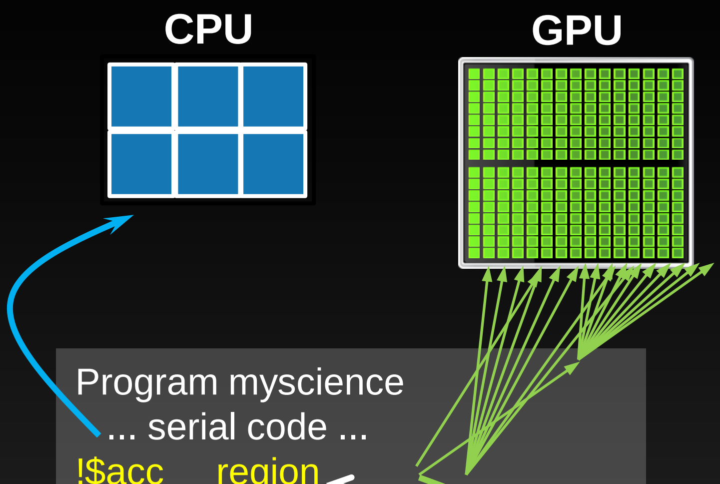
IMSL Library

Sparse Linear Algebra

Building-block Algorithms for CUDA

C++ STL Features for CUDA

OpenACC Directives




```
Program myscience
  ... serial code ...
!$acc   region
  do k = 1,n1
    do i = 1,n2
       ... parallel code ...
    enddo
   enddo
!$acc   end region
 ...
End Program myscience
```

OpenACC Compiler Hint

Your original Fortran or C code

Easy, Open, Powerful

- Simple Compiler hints
- Works on multicore CPUs & many core GPUs
- Compiler Parallelizes code
- Future Integration into OpenMP standard planned

http://www.openacc-standard.org

NVIDIA CRAY THE SUPERCOMPUTER COMPANY PGI CAPS

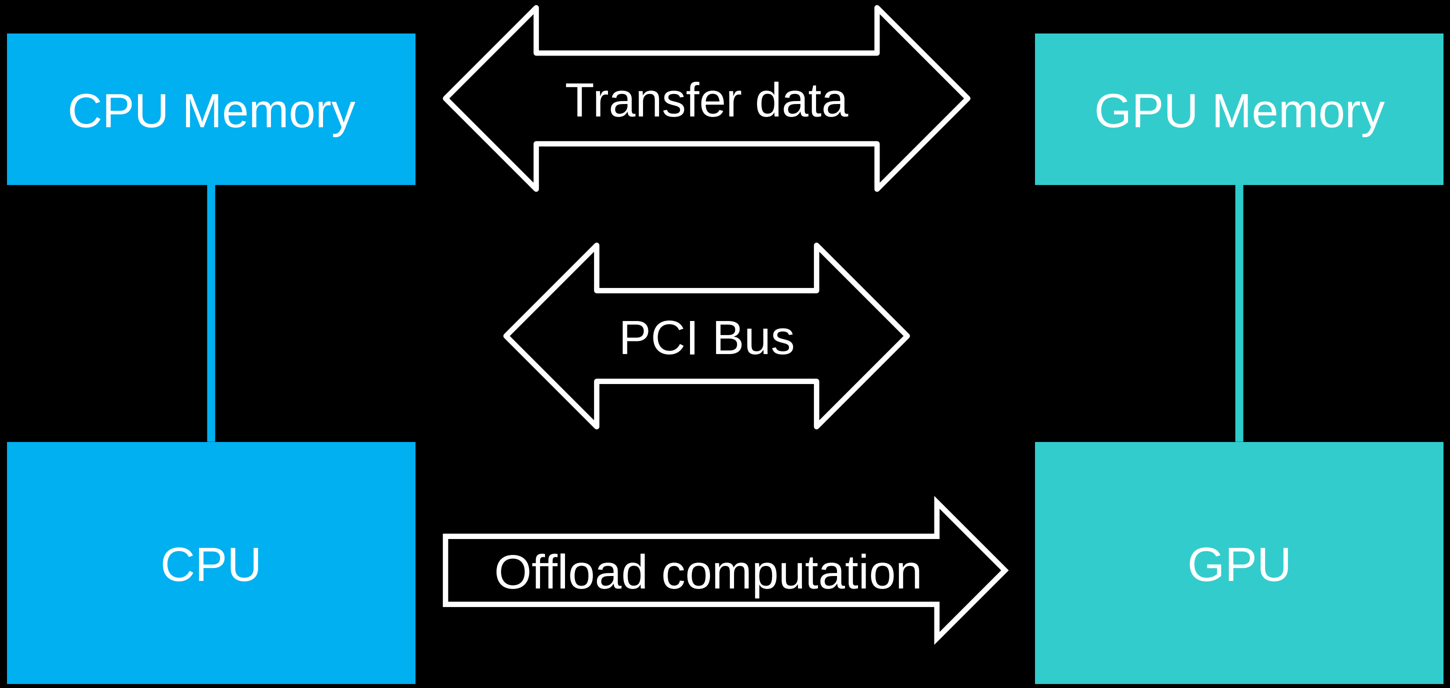
OpenACC

- Compiler directives to specify parallel regions in C, C++, Fortran
  - OpenACC compilers offload parallel regions from host to accelerator
  - Portable across OSes, host CPUs and accelerators

- Create high-level heterogeneous programs
  - Without explicit accelerator initialization,
  - Without explicit data or program transfers between host and accelerator

- Programming model allows programmers to start simple
  - Enhance with additional guidance for compiler on loop mappings, data location, and other performance details

Basic Concepts



For efficiency, decouple data movement and compute off-load

Directive Syntax

- Fortran

  !$acc directive [clause [,] clause] …]

  Often paired with a matching end directive surrounding a structured code block

  !$acc end *directive*

- C

  #pragma acc *directive [clause [,] clause] …]*

  Often followed by a structured code block

OpenACC Directive Set

- Parallel Constructs
  - #pragma acc parallel [clause [[,] clause]…] new-line
- Data Constructs
  - #pragma acc data [clause [[,] clause]…] new-line
- Loop Constructs
  - #pragma acc loop [clause [[,] clause]...]new-line
- Runtime Library Routines
- Cache Directives

- And few others…

Jacobi Relaxation

Iterate until converged

Iterate across elements of matrix

Calculate new value from neighbours

```
iter = 0
do while ( err .gt tol .and. iter .gt. iter_max )

  iter = iter + 1
  err = 0.0

  do j=1,m
    do i=1,n
      Anew(i,j) = 0.25 * (A(i+1,j) + A(i-1,j) + A(i,j-1) + A(i, j+1)
      err = max( err, abs(Anew(i,j)-A(i,j)) )
    end do
  end do

  if( mod(iter,100).eq.0 .or. iter.eq.1 ) print*, iter, err
  A = Anew
end do
```

OpenMP CPU Implementation

```
iter = 0
do while ( err .gt tol .and. iter .gt. iter_max )

  iter = iter + 1
  err = 0.0
!$omp parallel do shared(m,n,Anew,A) reduction(max:err)
  do j=1,m
    do i=1,n
      Anew(i,j) = 0.25 * (A(i+1,j) + A(i-1,j) + A(i,j-1) + A(i,  j+1)
      err = max( err, abs(Anew(i,j)-A(i,j)) )
    end do
  end do
!$omp end parallel do
  if( mod(iter,100).eq.0 ) print*, iter, err
  A = Anew
end do
```

Parallelise code inside region

Close off region

OpenACC GPU Implementation

```
!$acc data copy(A,Anew)
iter = 0
do while ( err .gt tol .and. iter .gt. iter_max )

  iter = iter + 1
  err = 0.0
!$acc parallel reduction( max:err )
  do j=1,m
    do i=1,n
      Anew(i,j) = 0.25 * (A(i+1,j) + A(i-1,j) + A(i,j-1) + A(i,j+1)
      err = max( err, abs(Anew(i,j)-A(i,j)) )
    end do
  end do
!$acc end parallel
  if( mod(iter,100).eq.0 ) print*, iter, err
  A = Anew
end do
!$acc end data
```

Copy arrays into GPU memory within region

Parallelise code inside region

Close off parallel region

Close off data region, copy data back

Improved OpenACC GPU Implementation

Reduced data movement

```
!$acc data copyin(A), copyout(Anew)
iter = 0
do while ( err .gt tol .and. iter .gt. iter_max )

  iter = iter + 1
  err = 0.0
!$acc parallel reduction( max:err )
  do j=1,m
    do i=1,n
      Anew(i,j) = 0.25 * ( A(i+1,j  ) + A(i-1,j  ) &
                           A(i,  j-1) + A(i,  j+1)
      err = max( err, abs(Anew(i,j)-A(i,j)) )
    end do
  end do
!$acc end parallel
  if( mod(iter,100).eq.0 ) print*, iter, err
  A = Anew
end do
!$acc end data
```

More Parallelism

```
!$acc data copyin(A), create(Anew)
iter = 0
do while ( err .gt. tol .and. iter .gt. iter_max )

  iter = iter + 1
  err = 0.0
!$acc parallel reduction( max:err )
  do j=1,m
    do i=1,n
      Anew(i,j) = 0.25 * ( A(i+1,j  ) + A(i-1,j  ) &
                           A(i,  j-1) + A(i,  j+1) )
      err = max( err, abs(Anew(i,j)-A(i,j)) )
    end do
  end do
!$acc end parallel
  if( mod(iter,100).eq.0 ) print*, iter, err
!$acc parallel
  A = Anew
!$acc end parallel
end do
!$acc end data
```

Anew now only exists on GPU

Find maximum over all iterations

Add second parallel region inside data region

More Performance

```
!$acc data copyin(A), create(Anew)
iter = 0
do while ( err .gt. tol .and. iter .gt. iter_max )

  iter = iter + 1
  err = 0.0
!$acc kernels loop reduction( max:err ), gang(32), worker(8)
  do j=1,m
    do i=1,n
      Anew(i,j) = 0.25 * ( A(i+1,j  ) + A(i-1,j  ) &
                           A(i,  j-1) + A(i,  j+1) )
      err = max( err, abs(Anew(i,j)-A(i,j)) )
    end do
  end do
!$acc end kernels loop
  if( mod(iter,100).eq.0 ) print*, iter, err
!$acc parallel
  A = Anew
!$acc end parallel
end do
!$acc end data
```

30% faster than default schedule

OpenACC: Small Effort, Real Impact

Large Oil Company

3x in 7 days

Solving billions of equations iteratively for oil production at world's largest petroleum reservoirs

Univ. of Houston

Prof. M.A. Kayali

20x in 2 days

Studying magnetic systems for innovations in magnetic storage media and memory, field sensors, and biomagnetism

Uni. Of Melbourne

Prof. Kerry Black

65x in 2 days

Better understand complex reasons by lifecycles of snapper fish in Port Phillip Bay

Ufa State Aviation

Prof. Arthur Yuldashev

7x in 4 Weeks

Generating stochastic geological models of oilfield reservoirs with borehole data

GAMESS-UK

Dr. Wilkinson, Prof. Naidoo

10x

Used for various fields such as investigating biofuel production and molecular sensors.

CUDA 4.1 Highlights

Advanced Application Development

- New LLVM-based compiler
- 3D surfaces & cube maps
- Peer-to-Peer between processes
- GPU reset with nvidia-smi
- New GrabCut sample shows interactive foreground extraction
- New code samples for optical flow, volume filtering and more…

GPU-Accelerated Libraries

- 1000+ new imaging functions
- Tri-diagonal solver 10x faster vs. MKL
- MRG32k3a & MTGP11213 RNGs
- New Bessell functions in Math lib
- 2x faster matrix-vector w/ HYB-ELL
- Boost-style placeholders in Thrust
- Batched GEMM for small matrices

New & Improved Developer Tools

- Re-Designed Visual Profiler
- Parallel Nsight 2.1
- Multi-context debugging
- assert() in device code
- Enhanced CUDA-MEMCHECK

New LLVM-based CUDA Compiler

- Delivers up to 10% faster application performance
- Faster compilation for increased developer productivity
- Modern compiler with broad support
  - Will bring more languages to the GPU
  - Easier to support CUDA to more platforms

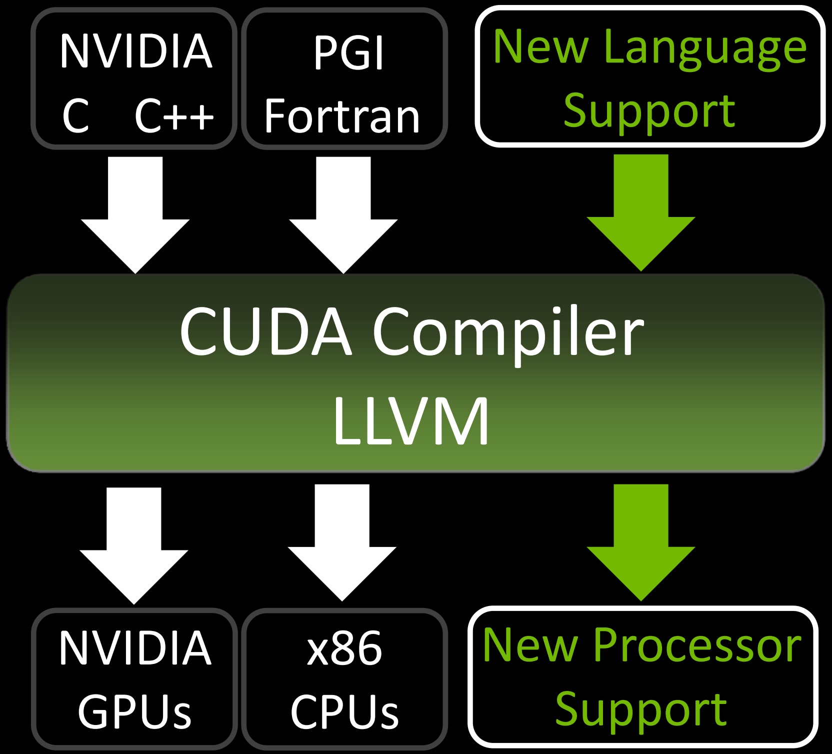
NVIDIA Opens Up CUDA Platform

CUDA Compiler Source for Researchers & Tools Vendors

Enables

New Language Support

New Processor Support



Apply for early access at
http://developer.nvidia.com/cuda-source

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May 14-17 | San Jose, CA

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- Explore the research as well as the commercial applications
- Discover advances in computational visualization
- Take a deep dive into parallel programming

Ways to participate

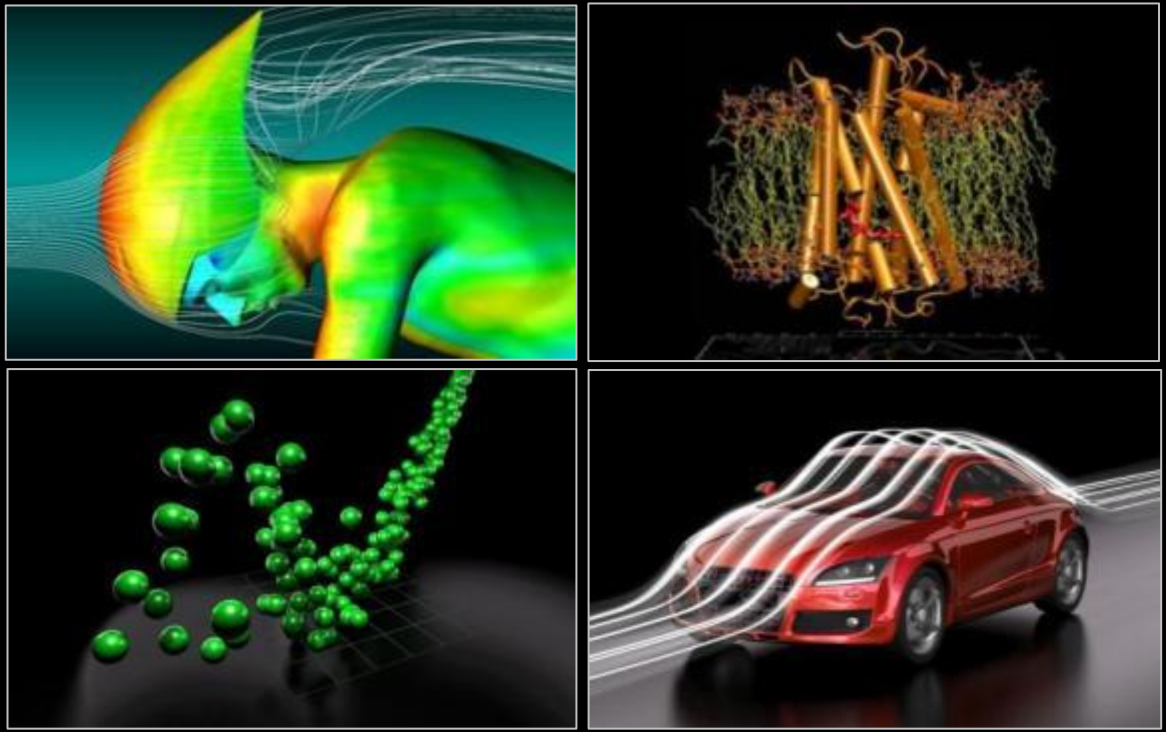
- Speak – share your work and gain exposure as a thought leader
- Register – learn from the experts and network with your peers
- Exhibit/Sponsor – promote your company as a key player in the GPU ecosystem

www.gputechconf.com

Summary

- Heterogeneous/hybrid Computing is the future
- OpenACC Directives provide a standardized way to hybrid computing
  - Easy , Open and Powerful
- Use highly optimized GPU libraries
- Use CUDA for maximum performance

Don’t wait and start today !!



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