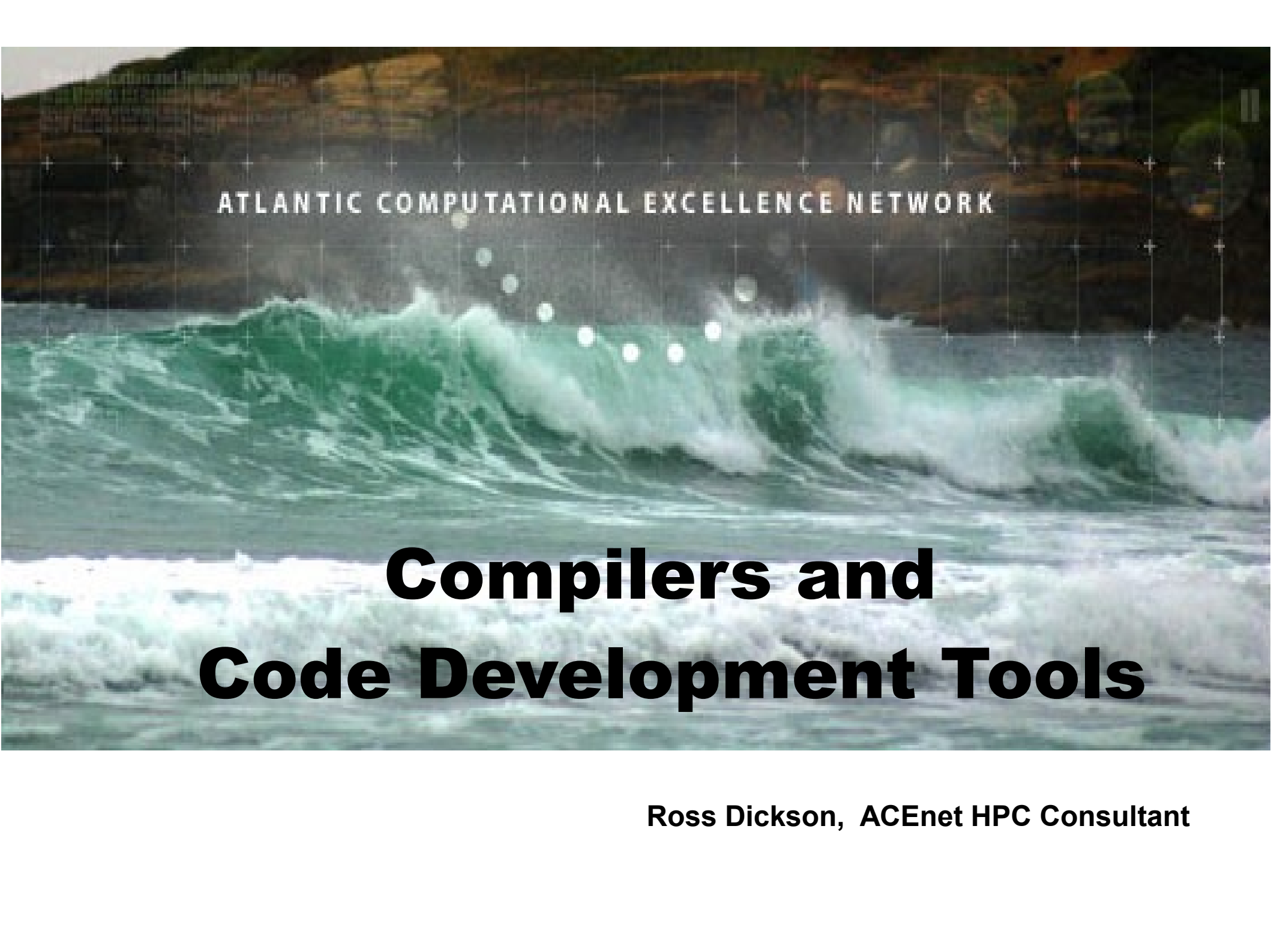




ATLANTIC COMPUTATIONAL EXCELLENCE NETWORK

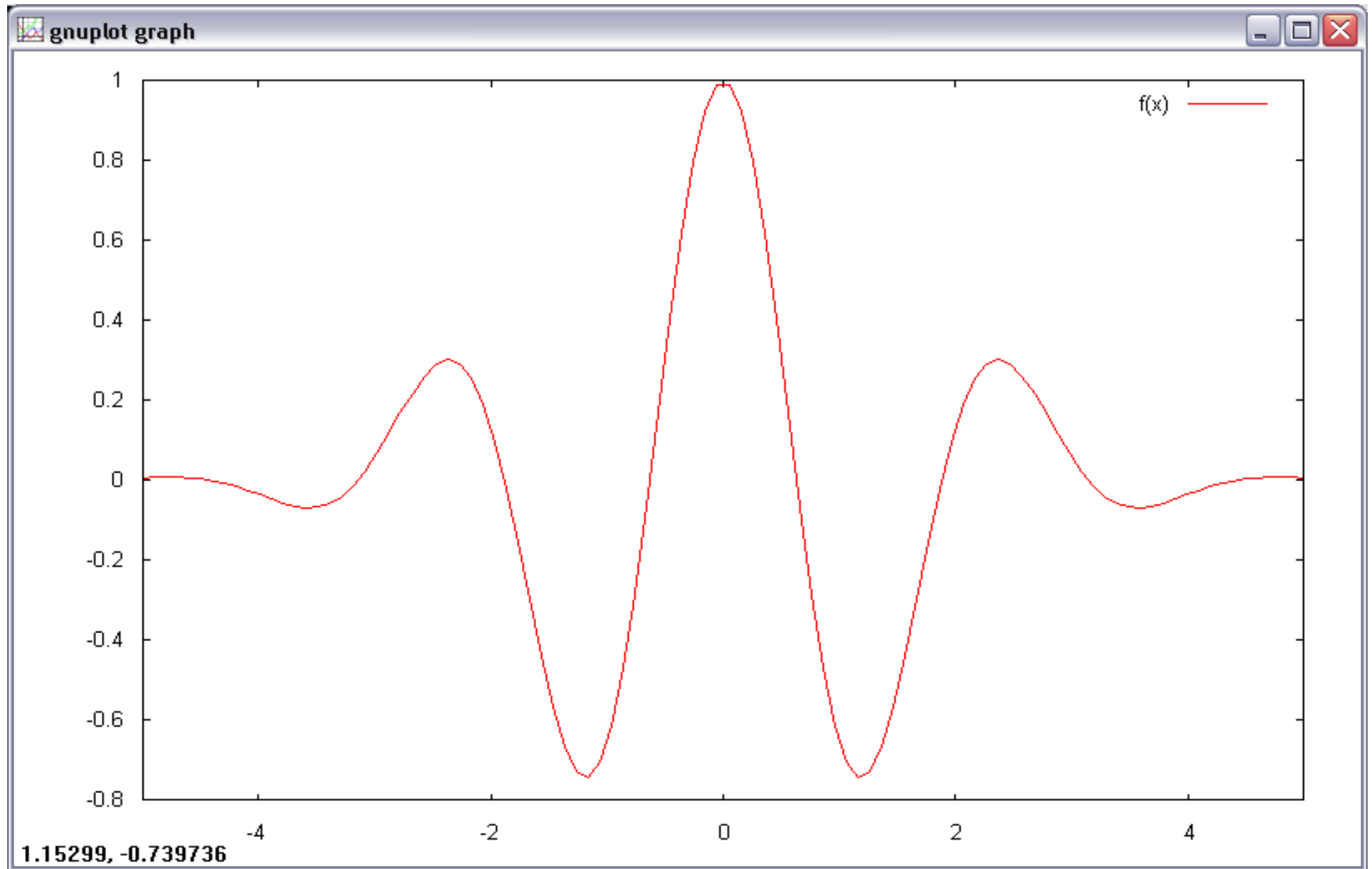
Compilers and Code Development Tools

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Compilers and Code Development

- Fortran, C, C++
- other languages
- command switches or 'flags'
- I/O redirection
- libraries
- Makefiles
- debugging

Integrate $f(x) = \exp(-0.2x^2)\cos(2.5x)$



Source code (Fortran)

```
program integrate
...
s = 0.0
do i=1,n
    x = (xleft - dx/2) + i*dx
    s = s + f(x)*dx
end do
...
function f(x)
real f,x
real, parameter :: a=0.2, b=2.5
f = exp(-a*x*x)*cos(b*x)
return
end function
...
```

Compile

```
> ls
biginput  infile          script
hello.c   integrate.f95
> f95 integrate.f95
> ls
a.out      hello.c          integrate.f95
biginput   infile           script
>
```

Run

```
> ls
```

```
a.out      hello.c    integrate.f95
```

```
biginput   infile     script
```

```
> a.out
```

```
a.out: Command not found.  pwd "." not in PATH !
```

```
> ./a.out  name it explicitly
```

```
Enter no. of intervals and right and left in
```

Compile and run

```
> f95 integrate.f95
```

```
> ./a.out
```

```
Enter no. of intervals and right and left in  
250 -2.0 2.0
```

```
Integrating over 250 points
```

```
between -2.0 and 2.0
```

```
Interval: 0.016
```

```
Integral: -0.35680311
```

```
>
```

Compile and run C

```
> cat hello.c
#include <stdio.h>

void main()
{
    printf ("Hello World!\n");
}

> cc hello.c
> ./a.out
Hello World!
>
```

Don't like “a.out”?

```
> mv a.out hello
> f95 integrate.f95 -o integrate
> ls
biginput          infile           script
hello            integrate
hello.c          integrate.f95
> ./hello
Hello World!
>
```

Compiler switches

- Also called “flags” or “options”
- Vary with compiler vendor
- Some common useful switches:
 - o <*file*> name output (executable) file
 - fast optimize for speed
 - g prepare for debugging
 - v or -# “verbose” – tell me everything
 - flags or --help list recognized options

Know your compiler!

```
> which cc
/opt/sun/sunstudio12/bin/cc
> which f95
/opt/sun/sunstudio12/bin/f95
> cc -flags | more
...
> man cc
...
```

Available compilers at ACEnet

C, C++, and Fortran

- Portland Group (PGI) version 8
 - `pgcc`, `pgCC`, `pgf77`, `pgf90`, `pgf95`
- GNU suite versions 3 and 4
 - `gcc`, `g++`, `gcc4`, `g++4`, `gfortran`, `g77`
- Intel Compiler Suite XE 2011
 - `icc`, `icpc`, `ifort`
- SunStudio version 12
 - `cc`, `CC`, `f77`, `f90`, `f95`

See <http://www.ace-net.ca/wiki/Compilers> for setup information

Other Available Languages

- **Ada (gnat)**
- **Java**
- **R**
- **Prolog**
- **Python**
- **Perl**
- **Ruby**
- **Octave**
- **...**

I/O redirection

```
> cat infile  
250 -2.0 2.0  
> integrate <infile >outfile  
>
```

I/O redirection

```
> cat infile
250  -2.0  2.0
> integrate <infile >outfile
> cat outfile
Enter no. of intervals and left and right
integration limits:
Integrating over 250 points
between -2.0 and 2.0
Interval: 0.016
Integral: 0.41237303
>
```

Libraries

- Collections of precompiled functions or subroutines
- Linear algebra, Fourier transforms, special functions, sorting, fast math, parallel programming, *et multae cetera*
 - http://www.ace-net.ca/wiki/Available_Software
- Typical usage:
 - > `f95 prog.f95 -lblas`
 - > `cc prog.c \`
 `-I/usr/local/netCDF/include \`
 `-L/usr/local/netCDF/lib -lnetcdf`

'make' and Makefiles

- Code may be spread across several files, require multiple libraries, compilation flags, *etc.*

```
> f90 -fast -g -llapack -lblas \  
    lebedev.f headers.f input.f xc.f \  
    scfnum.f scfnumx.f parnum.f -o parnum
```

- May require frequent recompilation during development
- Solution: 'make'
 - widely used throughout Unix/Linux community
 - Makefile contains compilation instructions
 - command 'make' reads local Makefile and calls compilers

Example Makefile

```
FFLAGS = -fast -g
LIBS = -llapack -lblas
OBJS = headers.o input.o xc.o parnum.o
parnum: $(OBJS)
    f90 $(FFLAGS) $(LIBS) $(OBJS) \
    -o parnum
```

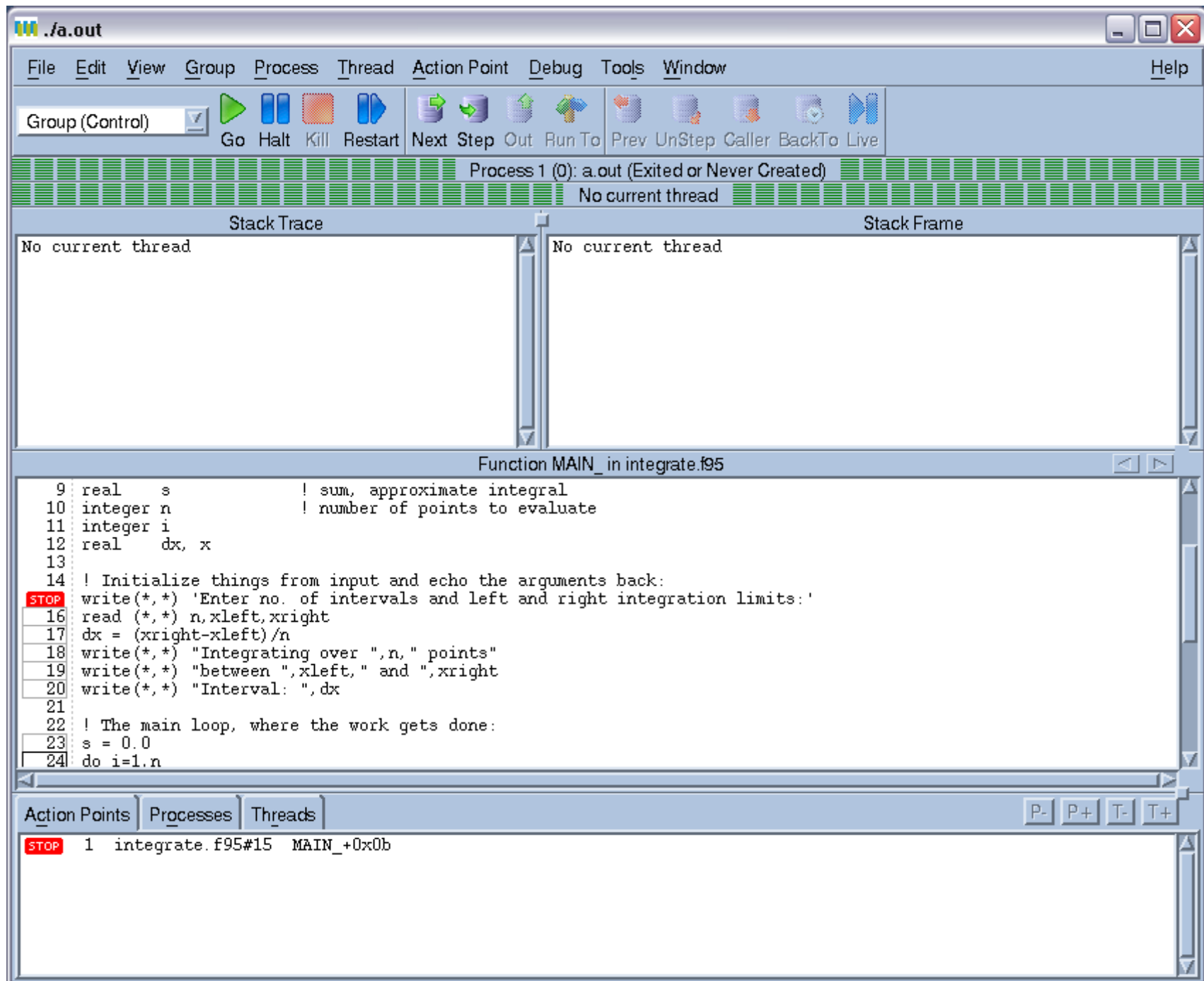
Invocation:

```
> make parnum
```

<http://www.gnu.org/software/make/manual/>

Debugging tools

- Command line tools
 - **`gdb`**, **`dbx`**
- Graphical debuggers for parallel code
 - `pgdbg` *with PGI compilers*
 - <http://www.ace-net.ca/wiki/Pgdbg>
 - TotalView
 - <http://www.ace-net.ca/wiki/TotalView>



MPI

"Message Passing Interface" – parallel programming

```
> mpf90 ftn_source -o mpi_executable  
> mpcc C_source -o mpi_executable  
> mpCC C++_source -o mpi_executable  
> mpirun -np n ./mpi_executable
```

PGI compilers underly the MPI compiler “wrappers”,
so see PGI documentation for flags

<http://www.ace-net.ca/wiki/MPI>

OpenMP

"Open MultiProcessing" – Shared-memory parallelism

```
> f90 -openmp -O3 omp_source -o omp_executable  
> cc -openmp -O3 omp_source -o omp_executable  
> setenv OMP_NUM_THREADS n  
> ./omp_executable
```

Different flags for different compilers:

`-openmp` (*Sun*) `-mp` (*PGI*) `-fopenmp` (*GNU*)

<http://www.ace-net.ca/wiki/OpenMP>

Where to go for help

- **man *command***
- Vendor sites:
 - <http://www.pgroup.com/resources/index.htm>
 - <http://www.gnu.org/software/gcc/>
 - <http://software.intel.com/en-us/articles/intel-composer-xe/>
 - <http://www.totalviewtech.com>
- ACEnet User Wiki
 - <http://www.ace-net.ca/>
- User support line
 - mailto: support@ace-net.ca

Want the example files?

```
mahone> mkdir workshop  
mahone> cd workshop  
mahone> cp /home/rdickson/demo/Coding/* .  
mahone> ls  
  
biginput          infile            script  
hello.c           integrate.f95  
mahone>
```