
CTC

Cornell Theory Center

Cornell University, Ithaca New York
Leading Edge Scalable Clusters

CTC-Manhattan, New York City
Clusters for Finance and Business Solutions

Over 100 Cornell Projects from Diverse Fields

- *Agricultural, Resource, and Managerial Economics*
- *Animal Science*
- *Astronomy*
- *Biochemistry, Molecular and Cell Biology*
- *Chemistry*
- *Chemical Engineering*
- *Civil and Environmental Engineering*
- *Clinical Sciences*
- *Computer Science*
- *Design and Environmental Analysis*
- *Ecology and Systematics*
- *Electrical Engineering*
- *Geological Sciences*
- *Marketing*
- *Mathematics*
- *Mechanical and Aerospace Engineering*
- *Neurobiology and Behavior*
- *Nuclear Science and Engineering*
- *Physics*
- *Plant Breeding and Biometry*
- *Theoretical and Applied Mechanics*

Key Components for Success

User Interfaces

- *Telnet – Seattle Lab and Microsoft built in.*
- *Cygwin, Interix – Unix tools + look and feel*
- *Terminal Server – Remote access to Windows GUI*
- *Citrix Terminal Server – Remote access to Windows GUI for non-MS platforms*
- *X Windows*

Ease of Porting from Other Environments

- *Compilers - MS, Compaq, Intel, PGI, Gnu*
- *Cygwin – Unix shell support and Make*
- *Debugging – Studio, Gnu*
- *MPIPro, MPI Software Technology, Inc.*

Batch and Interactive Job Scheduling

- *Cluster CoNTroller, MPI Software Technology, Inc.*

Reliable Servers, Software, and Storage

- *Windows 2000 Advanced Server – Solid!*
- *Dell Hardware – just works!*
- *Scalable Storage using Microsoft DFS.*

System Management

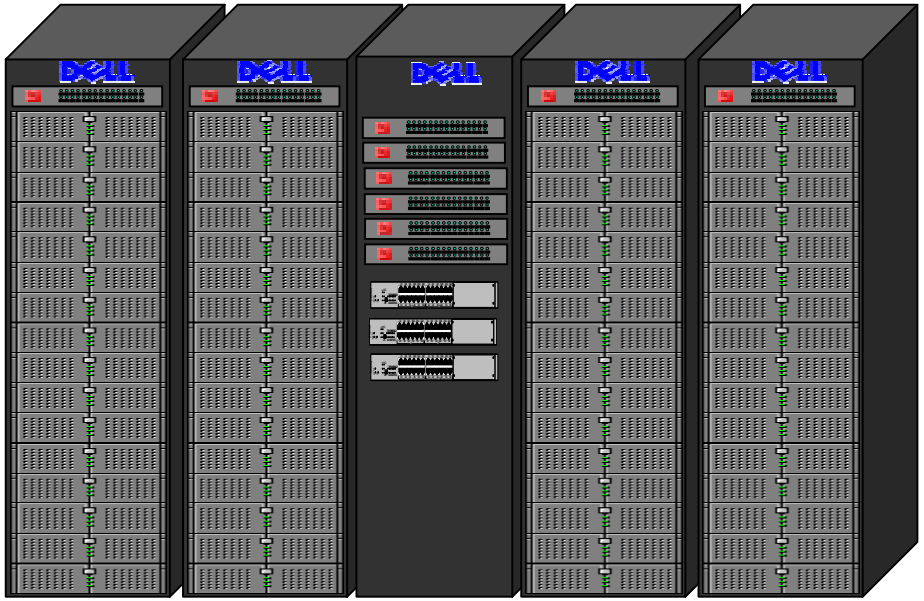
- *Windows Management Instrumentation*
- *CTC Domain Monitoring Tools*
- *Software Distribution and Remote Installation*

Velocity 1 – 256 Processors

64 Dell PowerEdge 6350 Servers

- *Quad Pentium III Xeon 500 Mhz (SMP)*
- *4 GB RAM/Node*
- *2 MB Cache/Processor*
- *50 GB Disk/Node (Raid 0 Stripe Set)*
- *Emulex CLan Interconnect (100 MB/second)*
- *Switched Ethernet (100 Mb/second)*

Velocity 1 Plus Cluster - 128 Processors



64 Dell PowerEdge 2450 Servers

- *Dual Pentium III 733 Mhz*
- *2 GB RAM/Node*
- *256 KB Cache/Processor*
- *27 GB Disk (RAID 0)/Node*
- *Emulex CLan Interconnect (100 MB/second)*
- *Switched Ethernet (100 Mb/second)*

Special Purpose CTC Clusters

32 Dell PowerEdge 2450 Servers (Application Center - .Net)

- *Dual Processor Pentium III 933 Mhz*
- *256 KB Cache/Processor*
- *2 GB RAM/Node*
- *27 GB Disk (RAID 0)/Node*

8 Dell PowerEdge 1550 Servers (NASA/NYS Educluster)

- *Dual Processor Pentium III 1 Ghz*
- *256 KB Cache/Processor*
- *2 GB RAM/Node*
- *27 GB Disk (RAID 0)/Node*

8 Dell PowerEdge 1550 Servers Development Cluster, 16 processors

- *Dual Processor Pentium III 866 MHz*
- *256 KB Cache/Processors*
- *2 GB RAM/Node*
- *27 GB Disk (RAID 0)/Node*
- *Emulex CLan Interconnect (100 MB/second)*
- *15 Minute Job Limit*

36 Dell PowerEdge Servers (Serial Nodes)

- *Pentium III 600+ MHz*
- *256 KB Cache/Processor*
- *1 GB RAM/Node*
- *27 GB Disk (RAID 0)/Node*

Dedicated Clusters

ARS/USDA Cluster for Agricultural Bioinformatics, 48 processors

- *4 Dell PowerEdge 6300 Servers*
- *Quad Processor SMP 400 Mhz Pentium II Xeons, 1 GB Ram, 56 GB Disk*
- *8 Dell PowerEdge 6350 Servers*
- *Quad Processor SMP 550 Mhz Pentium III Xeons, 1 GB Ram, 54 GB Disk*
- *Gigabit switched Ethernet*
- *2 TB Dell Power Vault Storage Equipment*

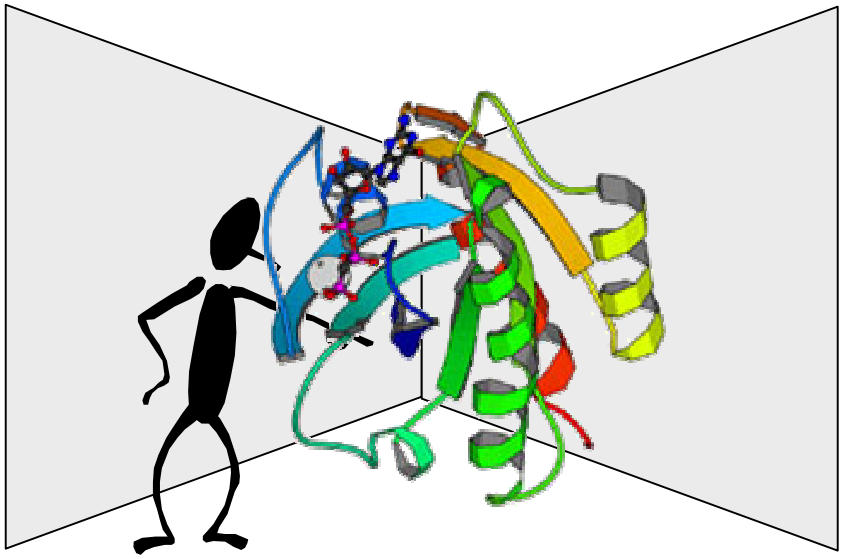
Social and Economics Research Cluster, 32 processors

- *8 Dell PowerEdge 6350 Servers*
- *Quad Processor SMP 550 Mhz Pentium III Xeons*
- *1 GB RAM/Node*
- *54 GB Disk/Node*
- *Gigabit switched Ethernet*
- *3 TB Dell Power Vault Storage Equipment*

Tri-Institutional/Computational Materials Institute Cluster, 256 processors

- *128 Dell PowerEdge 1550 Servers*
- *Dual Processor Pentium III 1 Ghz*
- *2 GB RAM/Node*
- *27 GB Disk (RAID 0)/Node*
- *Emulex CLan Interconnect*

Windows Based CAVE



- *3 Dual Processor Dell Precision 620 Workstations*
- *Wildcat 4210 Graphics Adapters*
- *1 GB RAM/Workstation*
- *Emulex CLan Interconnect*

Windows 2000 Cluster Management

Job Scheduling & Resource Management

Cluster CoNTroller

www.mpi-softtech.com/products/cluster_controller

Resource Monitoring

Windows Management Instrumentation

msdn.microsoft.com/library/en-us/dnwmi/html/wmicim.asp

Microsoft Operations Manager

www.microsoft.com/mom/

Perl & Python

www.activestate.com

System Installations

Symantec Ghost

enterprisesecurity.symantec.com/content/ProductJump.cfm?Product=3&PID=na

WinInstall LE

www.microsoft.com/WINDOWS2000/techinfo/planning/management/veritas.asp

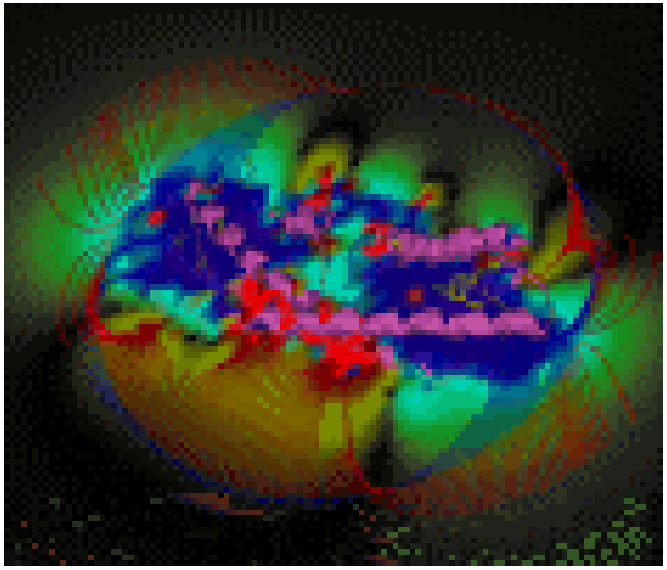
Reliability

CTC HPC Experience

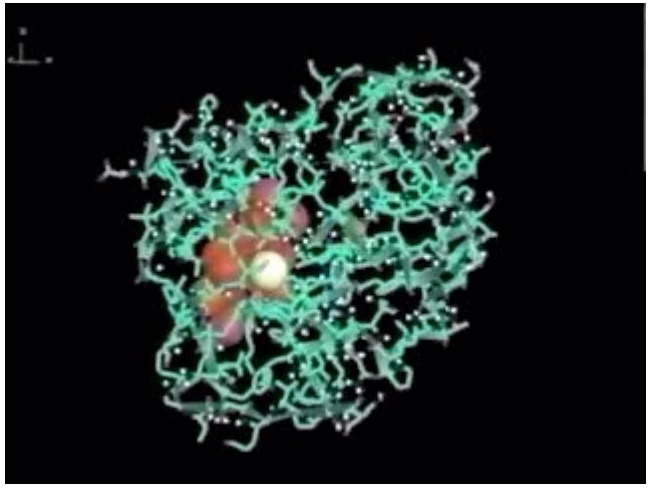
- ***99.9986% the first three months we ran Windows 2000***
- ***99.99999% the past four months!***
- ***Working on a Standard Reliability Benchmark***

Protein Folding/Structural Biology

Ron Elber, Harold Scheraga



Collaborators at Hauptman-Woodward Medical Research Institute; Mt. Sinai School of Medicine, U. Rochester



Cornell Faculty from Computer Science, Chemestry, and Biochemestry

Protein Folding Per/Processor Performance

Results on different computers for a protein structures:

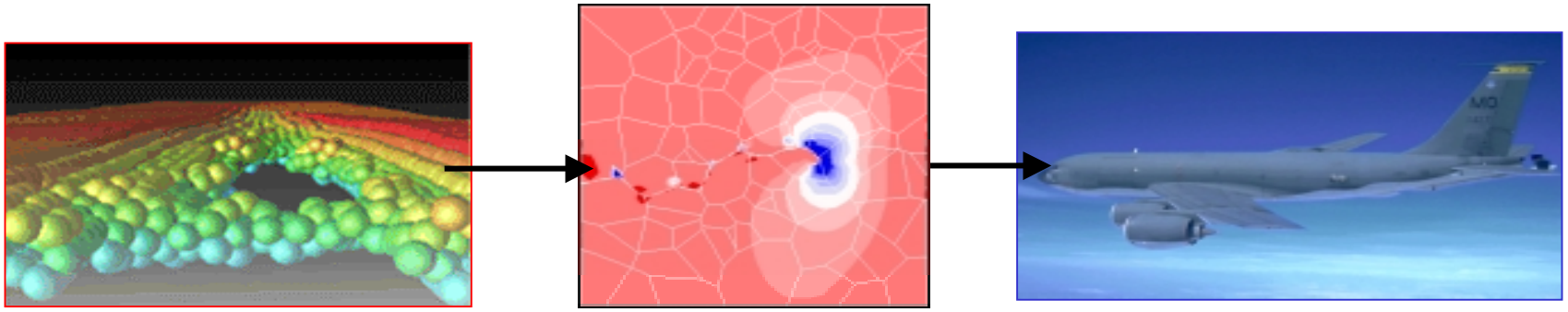
Machine	System	CPU	CPU speed [MHz]	compiler	Energy evaluations per second
Blue Horizon (SP San Diego)	AIX 4	Power3	222	xlf	44.3
Linux cluster	Linux 2.2	PentiumIII	650	PGF 3.1	59.1
Velocity (CTC)	Win 2000	PentiumIII Xeon	500	df v6.1	46.0
Velocity+ (CTC)	Win 2000	PentiumIII	733	df v6.1	59.2

Results on different computers for (a /b or b proteins):

Machine	System	CPU	CPU speed [MHz]	compiler	Energy evaluations per second
Blue Horizon (SP San Diego)	AIX 4	Power3	222	xlf	15.0
Linux cluster	Linux 2.2	PentiumIII	650	PGF 3.1	21.0
Velocity (CTC)	Win 2000	PentiumIII Xeon	500	df v6.1	16.9
Velocity+ (CTC)	Win 2000	PentiumIII	733	df v6.1	22.4

Computational Materials Institute

Anthony Ingraffea, Keshav Pingali



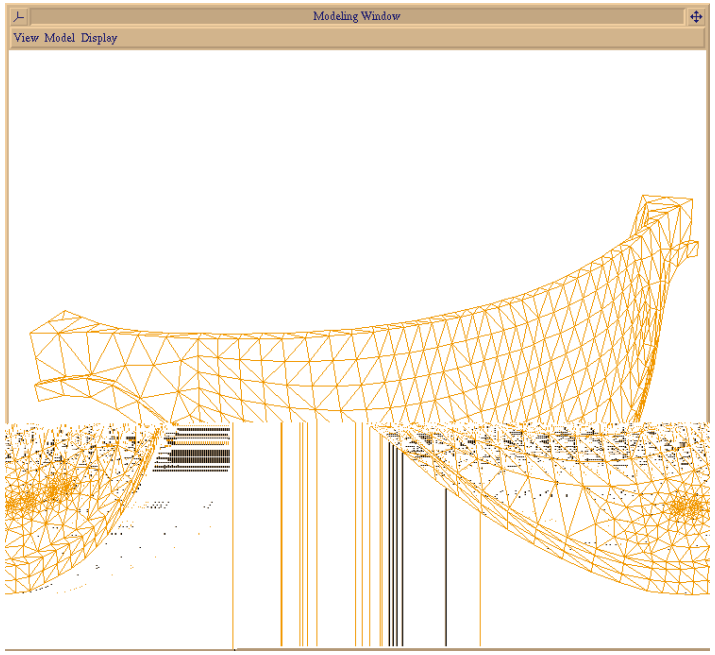
10^{-10} m 10^{-5} m 10^{2} m

Mission:

- ***Connect nano-scale and intermediate scale understanding of "old" materials to new designs and life-extension of existing designs;***
- ***Create simulation tools that support virtual design and testing of new materials;***
- ***Compliment the theoretical/experimental activities of the Cornell Center for Materials Research.***

Concrete Dam

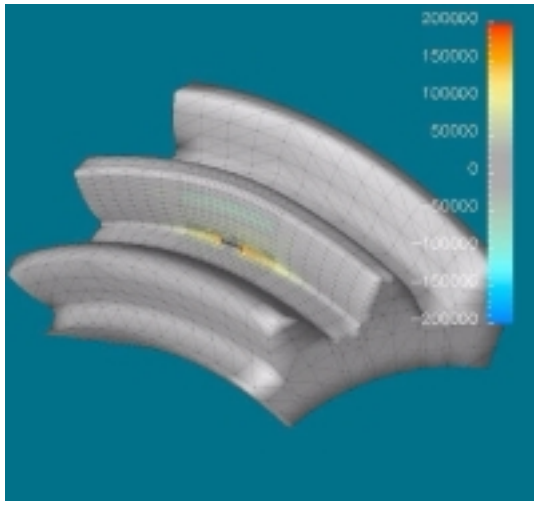
Vertices : 86,325 Tetrahedra : 401,124 dof



Machine	Processors	Time/Iteration
SP2	16x1	0.48
Velocity	4x4	0.53
Velocity	8x2	0.43
Velocity	16x1	0.39
SP2	32x1	0.27
Velocity	8x4	0.27
Velocity	16x2	0.22
Velocity	32x1	0.2
SP2	64x1	0.16
Velocity	16x4	0.15
Velocity	32x2	0.12
Velocity	64x1	0.12

Fatigue Cracks in Spiral Bevel Power Transmission Gear

Vertices : 344,777 Tetrahedra : 1,535,943 dof



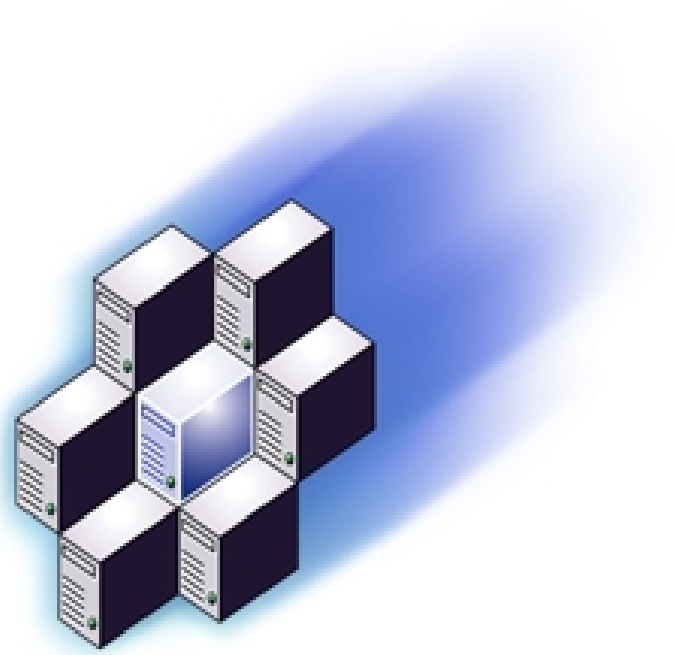
Machine	Processors	Time/Iteration
Velocity	16x1	1.54
Velocity	16x2	0.87
Velocity	32x1	0.78
Velocity	16x4	0.55
Velocity	32x2	0.44
Velocity	64x1	0.4
Velocity	20x4	0.43
Velocity	40x2	0.36
Velocity	64x2	0.23

Microsoft Application Center 2000

Bioinformatics

Fracture Mechanics

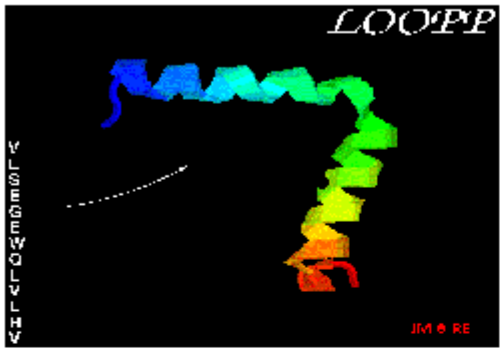
Finance



Microsoft .net

Learning, Observing and Outputting Protein Patterns (LOOPP)

by Jarek Meller and Ron Elber



The **LOOPP** program (Learning, Observing and Outputting Protein Patterns). A program for potential optimization and alignments. LOOPP aligns sequence to sequence, sequence to structure, and structure to structure. It further enables the optimization of potentials and scoring functions for the above mentioned applications.

To download the source code, click here
Click here for Loopp online tutorial

submit your sequence to our server, complete the requested information below, then click Submit/Run Prediction.
ur results will be sent to you by email at the address you provide.

pe the information into the fields	Description of field
	Your email address
	Name of sequence (optional)
	Paste, or type your sequence • amino acids in one-letter code • white spaces allowed • non-standard amino acids ignored • use SRS6 to get your sequence from a public database

SUBMIT / RUN PREDICTION CLEAR PAGE

ck to LOOPP Web Page

Computational Biology Service Unit

Cornell Theory Center — Cornell University

PDB code: QuickPDB | Local BLAST | NCBI BLAST | Workspace Bookmarks: Add, Edit, Open Window | Menu window, Save status, Hide Menu, Show Menu | Configured for default, Reset, Display Settings, He

- Home
- Software
- Education
- Web Computing
- Web Resources
- About us
- Contact CBSU
- Mailing list

Expand all | Restore all | Help

Welcome to the Computational Biology Service Unit at the Cornell Theory Center

send comments or questions about this site to the CBSU webmasters.

site is best viewed with Internet Explorer.

BLAST @ CBSU

Query Type: Nucleotide E-mail:

You will receive an e-mail with a link to your results once the blast search is submitted. The blast calculations will be carried out at the serial compute nodes cluster at the Cornell Theory Center.

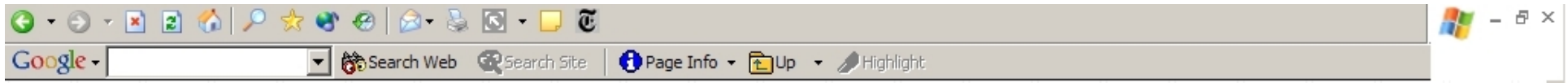
Paste your sequence here:

Or select the text file from your desktop computer (FASTA format):

Browse...

Choose Database for BLAST

Available: nt, est, ecoli.nt — add — del — Selected:

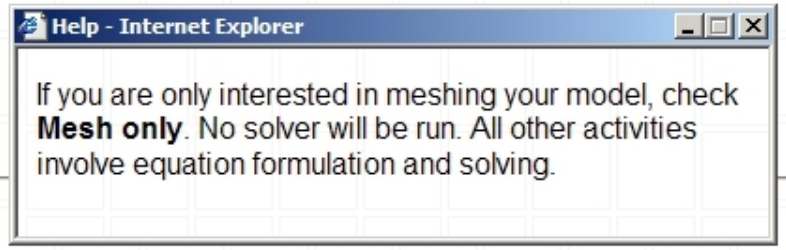


Welcome to the CPTC web-interface!

User Information

(You logged in as user: **CTC_ITH\heber**)

Username: **heber** Email Address: heber@tc.cornell.edu Help



General Information

Do you want to run an **analysis** on your model or just create a mesh for it? Help

(•) Analysis ( ) Mesh **only**

Does your model have **cracks** in it? Help

(•) Yes ( ) No

Do you want to have the crack grown **automatically** for some steps? Help

( ) Yes (•) No

Do you want to perform multiple **load steps**? Help

( ) Yes (•) No

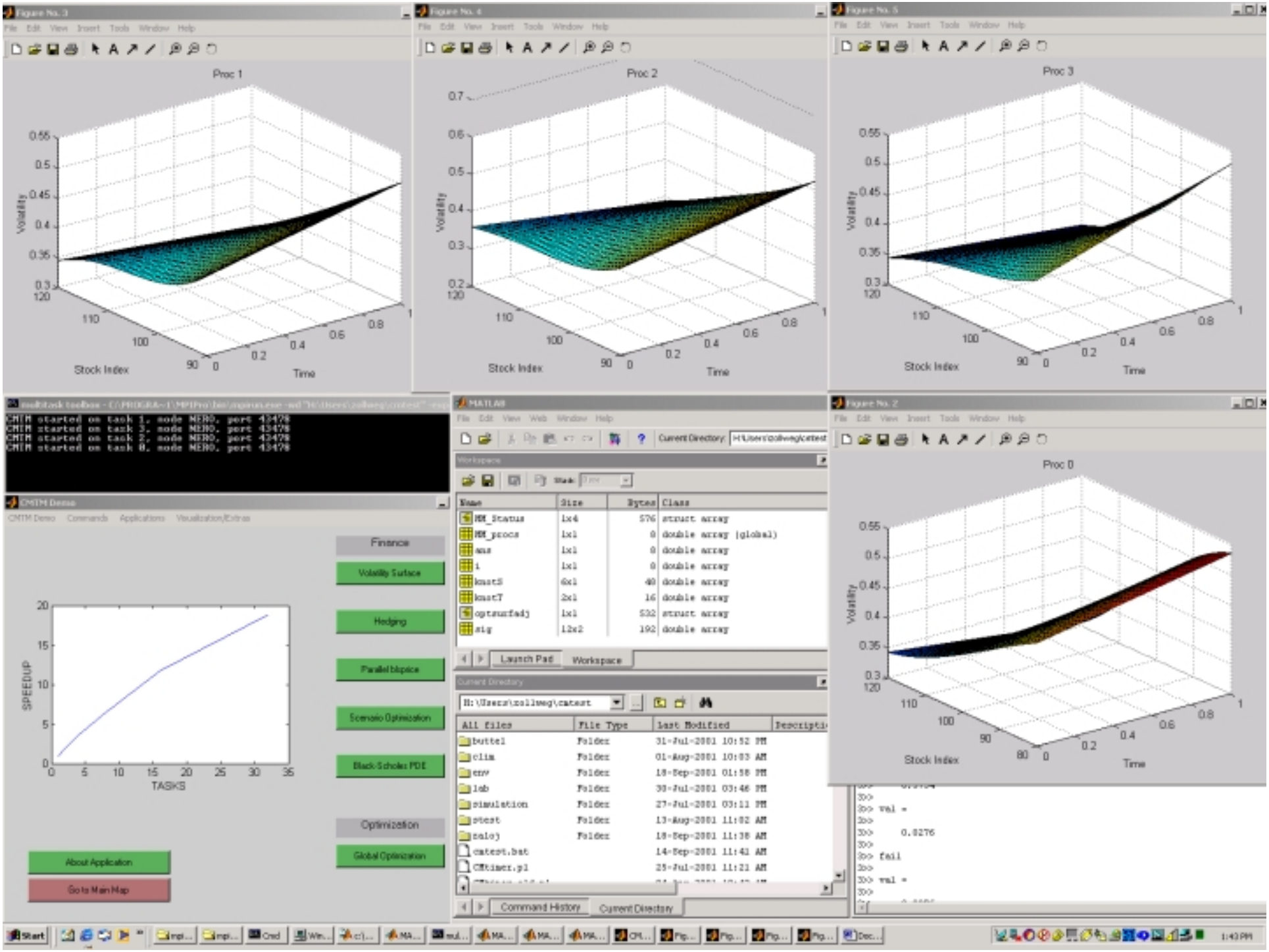
Where are your **executables** located? Help

H:\Users\heber\bin

Model Information

Model Name: model

Model Directory: H:\Users\heber\model Help


Proc 1
Proc 2
Proc 3
Proc 0
Volatility
Stock Index
Time
CMTM started on task 1, node NERO, port 43478
CMTM started on task 3, node NERO, port 43478
CMTM started on task 2, node NERO, port 43478
CMTM started on task 0, node NERO, port 43478
CMTM Demo
Finance
Volatility Surface
Hedging
Parallelspice
Scenario Optimization
Black-Scholes PDE
Optimization
Global Optimization
About Application
Go to Main Map
SPEEDUP
TASKS
MATLAB
Launch Pad
Workspace
Current Directory
Command History
Current Directory
val =
0.8276
fail
val =