TEXAS TECH UNIVERSITY
Information Technology Division

High Performance Computing Center

TIGRE: The Texas Grid Computing Infrastructure Project

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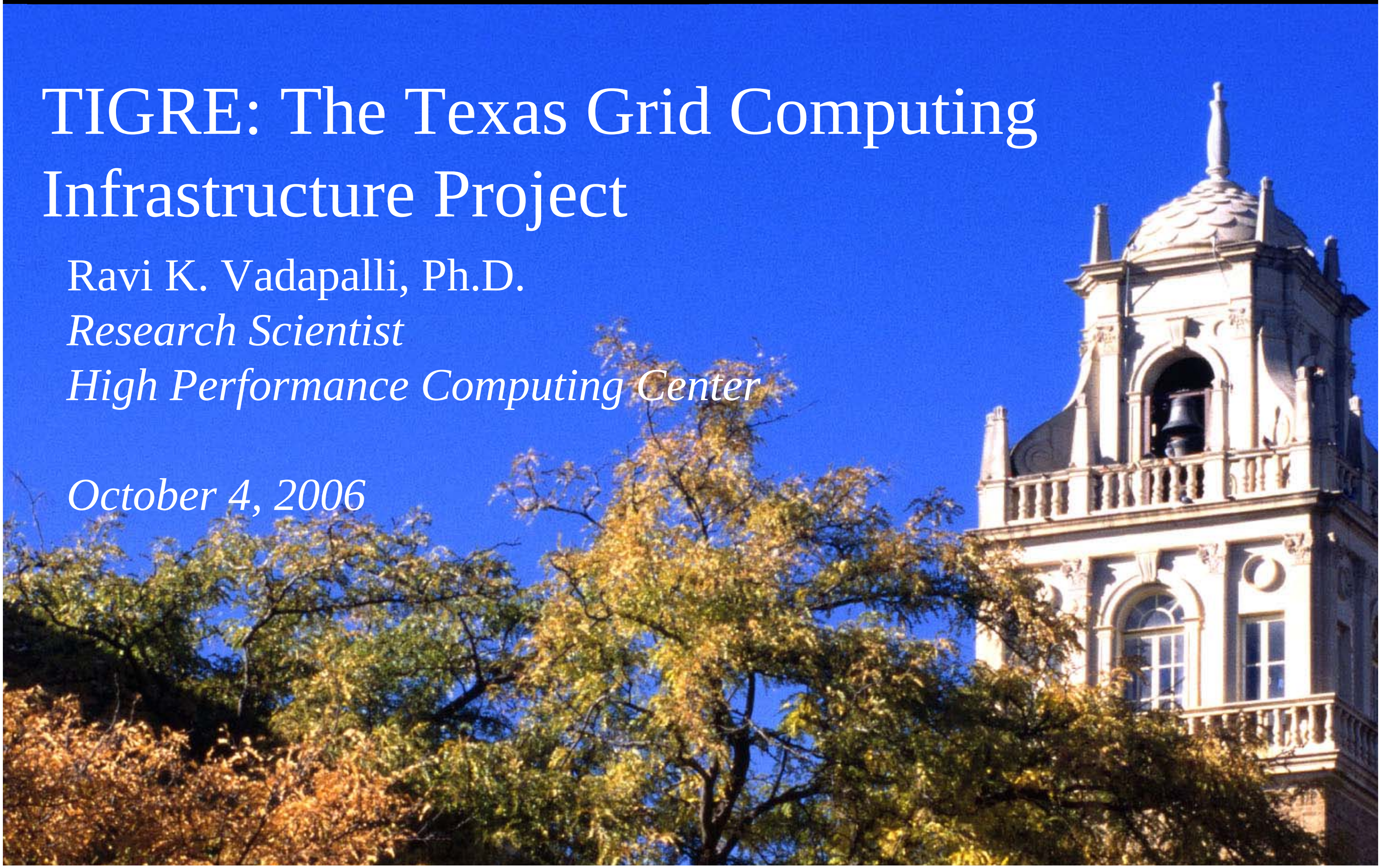
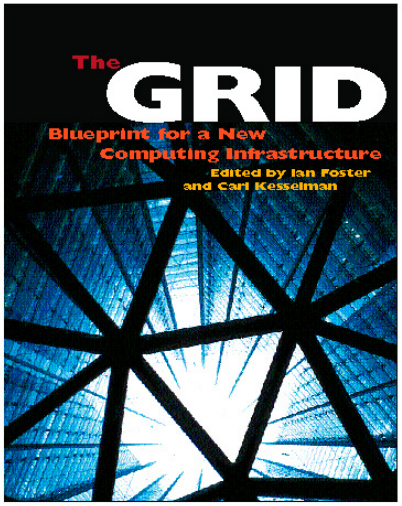


Grids are “**Hot**”



Data - Computation - Information - Access - Knowledge

But What Are They?

Collection of heterogeneous computing resources

- Computers, data repositories, networks, and tools
- Varying in power, architectures, and purpose

Distributed

- Across the room, campus, city, state, nation, globe

Complex (Today)

- Hard to program
- Hard to manage
- Interconnected by networks
  - *Links may vary in bandwidth*
  - *Load may vary dynamically*
  - *Reliability and security concerns*

BUT – The platform for next generation computational science and engineering!

TIGRE Project

Texas Internet Grid for Research and Education (TIGRE)

- TIGRE is a state funded project of the HiPCAT consortium.
- TIGRE is a construction project primarily between Rice, A&M, TTU, UH, and UT Austin.
- TIGRE is an “application driven” project targeted *primarily* to extend the computational scope in
  - *Bioscience and medicine*
  - *Energy and*
  - *Environment*

TIGRE Vision

Design and deploy state-of-the-art grid computing infrastructure to

- Enhance the research and educational capabilities
- Facilitate new modalities for Academic-government-private research partnerships.
- Foster advanced computing technology transfer to Texas companies/industry.
- Become national model for organizations serving higher education
- Competitive model for external funding.

TIGRE Infrastructure "Scope"

Application Users

- Compile & Debug codes
- Resource Selection
- Who to contact?
- Stage In/Out Data
- Job submission & Exec.
- Is my data secure?
- Application Mgmt. & Collaborations

Resource Providers

- GSI OpenSSH
- Web Portal
- TTS, CSM
- Grid/UberFTP, GridSCP
- WS-GRAM, Condor-G
- AuthZ/AuthN (MyProxy)
- Application VOs?
- Outreach/Tutorials, etc.

TIGRE: “Activity Driven”

Steering Committee:

- PIs from TIGRE Institutions.
- Defined Quarterly Milestones.
- Planning & Driving the Project direction.
- Meets periodically via F2F or teleconference.

Developers Team:

- Personnel funded through the TIGRE project.
- Milestones are divided into a set of project deliverables.
- The deliverables constitute one or more activities/sub-activities depending on the granularity of the task.
- Software stack, AuthN/AuthZ, Operations & Monitoring, Outreach, Reference Design, and Potential & Driving Applications.

TIGRE: “Milestones & Deliverables”

Project start date: Dec 1, 2005

YEAR 1
Q1:
Project plan ✓
Web site ✓
Certificate Authority ✓
Minimum testbed requirements ✓
Select 3 driving applications ✓
Q2:
Alpha portal ✓
Q3:
Define software stack ✓
Distribution Mechanism ✓
Simple demo of UltraScan from UTHSCSA (TIGRE app) ✓
Q4: IN PROGRESS …
Alpha client software distributed

YEAR 2
Q1:
Alpha customer management services system deployed & demonstrated
Q2:
Global grid scheduler deployed
Q3:
Stable software available (only bug fixes after this)
Required services TIGRE specified
Q4:
Complete hardening of software
Complete documentation
Finalized procedures and policies to join TIGRE & document
Demonstrate TIGRE at SC2007

... Making excellent progress!!

TIGRE Grid Middleware

Consists of two initial stacks – client stack and server stack, drawn from the VDT – web service based.

- Contents of the cluster/compute server stack
  - *Globus Toolkit 4.0 (Servers and clients)*
  - *Grid Proxy programs for obtaining TIGRE credentials*
  - *GSI OpenSSH, UberFTP, MyProxy, and Gondor-G*
  - *GPIR monitoring (added manually after the VDT pieces)*
- Contents of the client only software stack
  - *Globus Toolkit 4.0 clients (Grid Proxy programs, WS-GRAM client, and GridFTP client for secure, and high-bandwidth file transfers)*
  - *GSI OpenSSH client for compiling and debugging programs*
  - *UberFTP, MyProxy client for obtaining TIGRE credentials, and*
  - *Condor-G job scheduling and manangement*
- Grid Storage (Not resolved for TIGRE yet)

TIGRE Testbed

Sever Stack: VDT 1.3.10 based TIGRE stack is wrapped in the customized PacMan for TIGRE.

- Host and user grid certificates were issued by TACC.
- TIGRE Developers are provided with login accounts.
- User credentials are mapped manually to their login accounts.
- TIGRE Institutions contributed resources for TIGRE testbed.
- Grid Portal Information Repository (GPIR) service from TACC reports cluster status at the TIGRE portal http://tigreportal.hipcat.net
- TIGRE server stack is fully web-service based. XML is used to create job submission scripts.
- WS-GRAM interface for local job scheduler prepares the job submission script and launches the job on the scheduler.

TIGRE User Portal

Provided by TACC, similar to TeraGrid and SURAGrid Portals

TIGRE User Portal

Welcome | Resources | Documentation | Accounts & Allocations | Consulting | Feedback | Administrators

Resource Monitor

Grid Information Browser

Refresh

Parallel Computing Resources										
Name	Institution	Department	System	CPUs	Peak GFlops	Memory GBytes	Disk GBytes	Status	Load	Jobs
Bandera	The University of Texas at Austin	Texas Advanced Computing Center	TACC DGC Cluster	8	48	8	144	↑		0R-0Q-0O
Calclab	Texas A&M University	Department of Mathematics	Calclab Optiplex Cluster	223	1200	224	765	↑		0R-0Q-0O
Cosmos	Texas A&M University	Texas A&M Supercomputing Facility	SGI Altix	128	666	256	4096	↑		48R-60Q-0O
Lonestar	The University of Texas at Austin	Texas Advanced Computing Center	Dell Linux Cluster	1028	6291	1984	33736	↑		50R-0Q-76O
RTC	Rice University	Computer and Information Technology Institute	HP Itanium II Linux Cluster	290	1044	596	7000	↑		0R-0Q-0O
			Total:	**1677**	**9249**	**3068**	**45741**			

High Throughput Computing Resources									
Name	Institution	Department	System	Active PCs	Active CPUs	Memory GBytes	Disk GBytes	Resource Details	Jobs
glb-test	Texas Tech University	High Performance Computing Center	Condor	0 / 0	0 / 0	0	0		
Rodeo	The University of Texas at Austin	Texas Advanced Computing Center	Condor	387 / 764	62 / 65	1241	5299		
			Total:	**387 / 764**	**62 / 65**	**1241**	**5299**		

Jobs Key: **#R** - Number of Jobs Running, **#Q** - Number of Jobs Queued, **#O** - Number of Jobs in an Other State

Need to add your grid resource to the resource browser?

built with gridport

Typical Job submission script

```
<job>
  <executable>binary</executable>
  <directory>${GLOBUS_USER_HOME}/DEST-DIR</directory>
  <argument>-f</argument>
  <argument>input file</argument>
  <argument>output file</argument>
  <fileStageIn>
    <transfer>
      <sourceUrl>gsiftp://submission-hostname:2811/input file</sourceUrl>
      <destinationUrl>file:///${GLOBUS_USER_HOME}/inputfile</destinationUrl>
    </transfer>
  </fileStageIn>
  <fileStageOut>
    <transfer>
      <sourceUrl>file:///${GLOBUS_USER_HOME}/output file</sourceUrl>
      <destinationUrl>gsiftp://hostname:2811/output file</destinationUrl>
    </transfer>
  </fileStageOut>
</job>
```

Demo Application I: Proth

Proth's Theorem (1878): Let $N = h.2^k+1$ with $2^k > h$. If there is an integer a such that

$a^{(N-1)/2} = -1 \pmod N$, then N is prime. "a" is called the witness.

The goal of Proth code is to find largest prime in a given $[h_l:h_f, k]$ domain.

Importance: Large primes are of great importance in data encryption standards, and computer security. More info on Proth can be found at http://www.prothsearch.net

Proth is an ideally "grid suitable" application.

Algorithm:

1. Submit (h_i, k) pair to a processor,.
2. Collect all results into a DEST-DIR.
3. Search for primes in the list.

TIGRE Driving Applications

Bioscience & Medicine

1. UltraScan (TACC & UTHSCSA)
2. Computational Radiotherapy (TTHSC, JACC, SWCC, and MDACC)

New Directions in Radiotherapy

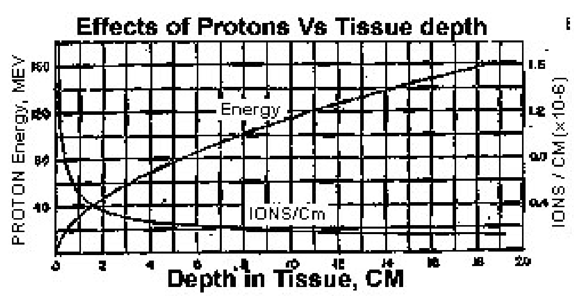
Radiological Use of Fast Protons

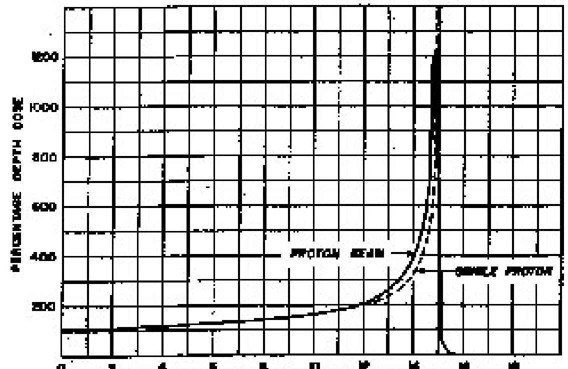
ROBERT R WILSON
Research Laboratory of Physics, Harvard University Cambridge, Massachusetts
Accepted for publication in July 1946.

Except for electrons, the particles which have been accelerated to high energies by machines such as cyclotrons or Van de Graaff generators have not been directly used therapeutically. Rather, the neutrons, gamma rays, or artificial radioactivities produced in various reactions of the primary particles have been applied to medical problems. This has, in large part, been due to the very short penetration in tissue of protons, deuterons, and alpha particles from present accelerators.

Higher-energy machines are now under construction, however, and the ions from them will in general be energetic enough to have a range in tissue comparable to body dimensions. It must have occurred to many people that the particles themselves now become of considerable therapeutic interest. The object of this paper is to acquaint medical and biological workers with some of the physical properties and possibilities of such rays.

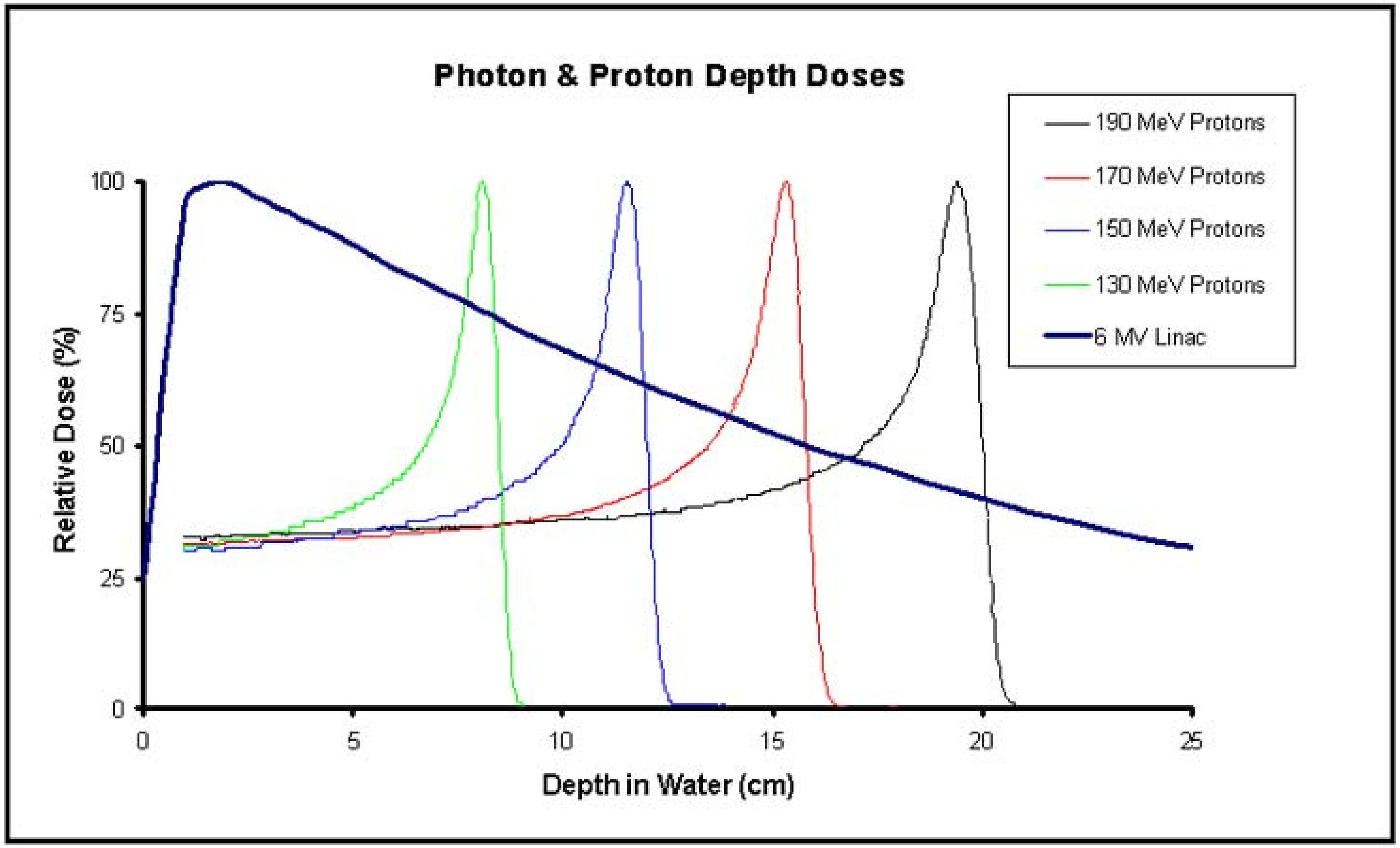
To be as simple as possible, let us consider only high-energy protons: later we can generalize to other particles. The accelerators now being constructed or planned will yield protons of energies above 125 MeV (million electron volts) and perhaps as high as 400 MeV. The range of a 125 MeV proton in tissue is 12 cm., while that of a 200 MeV proton is 27 cm. It is clear that such protons can penetrate to any part of the body.





Dosage due to 140 MEV Protons in tissue

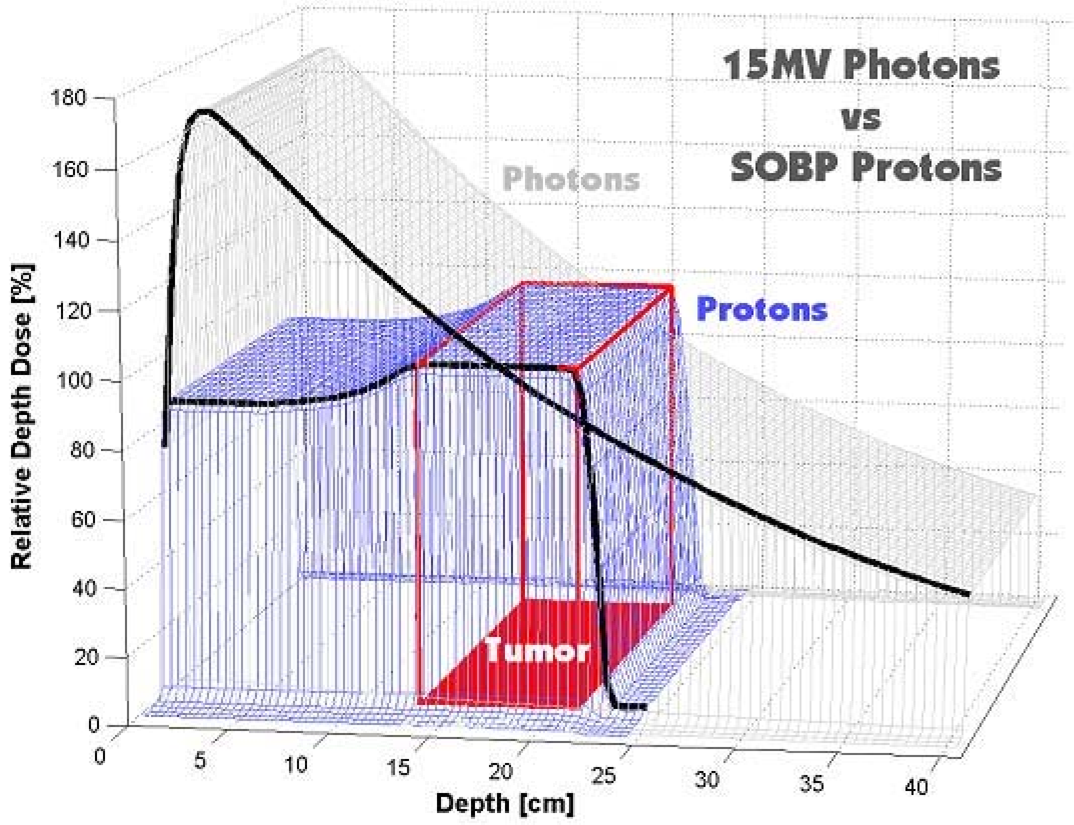
Proton Depth Doses



From MGH Website

Proton v. Photon Therapy

SOBP: Spread-out Bragg Peak



From MGH Website

Monte Carlo Transport Codes

Represent stochastic processes probabilistically using random number generators…

Simulate the motion of the particles through matter using known microscopic physics processes…

Require accurate knowledge of the physical geometry and material composition of the matter traversed…

"Score" energy deposited and calculate dose endpoints statistically for designated volumes within the geometry by running many incident trial particles.

Justification

Benchmark runs @ MD Anderson

- Monte Carlo simulation of water phantom using 250 MeV proton beams.
- A 60 3.0 GHz Pentium 4 processor cluster, 200 M particle histories, 2D geometry.
- Runtime: eight hours, 2% - 4% uncertainty.

Simple Math

- Facility cost: $125 M. Cost effective treatment requires 300-350 patients day.
- Less than half-an-hour per patient (assuming 5 gantries).

Target

- 1000 Pentium 4 processors are required for 2D simulations.

Pilot Project: HDR Branchy Vs. Proton

Code sets: FLUKA, GEANT4, MCNP.

Collaboration: MDACC, UH, JACC, and TTU.

Future Directions

- Software toolkit for treatment planning.
- Potential industrial collaborations.
- Data security.
- Classroom demonstrations & educational outreach.
- Medical Physics program.

Summary

- TIGRE is an “application driven” grid computing infrastructure development project.
- TIGRE is targeted to mitigate computational challenges in three driving application areas of interest to the state of Texas. They are (1) Bioscience and medicine (2) energy and (3) environment.
- TIGRE adopted “activity driven” top-down approach to meet the milestones determined by the project PIs (the Steering Committee).
- The ultimate goal of TIGRE is to connect with the national grid projects such as TeraGrid, and OSG. Its future directions include
  - *Expansion to involve other Texas institutions beyond the primary five.*
  - *Identify new applications and their grid suitability, and explore setting up of application VOs (OSG approach).*
  - *Extend scientific scope by recruiting interdisciplinary applications.*
  - *Competitive model for advanced computing in institutions primarily engaged in higher education.*