Research and Education with and in State-of-the-art Networking

Lennart Johnsson
Director, the Texas Learning and Computation Center
Cullen Distinguished Professor of Computer Science, Mathematics and Electrical and Computer Engineering

Texas Learning & Computation Center
Outline

- The Texas Learning and Computation Center
- UH Research Needing High-End Networking
UHResearch needing high-end networking (examples)

- Chemistry (Dr Montgomery Pettitt, Director, Institute for Molecular Design, in Mexico)
- Computer Science and Engineering, Dr Driss Benhaddou
- Environmental Science, Dr Daewon Byun, Director, Institute for Multidimensional Air Quality Studies
- Life Sciences
- Petroleum exploration (Dr Arthur Weglein, Director, Mission Oriented Seismic Research Program, in Saudi Arabia)
- Physics (Dr Larry Pinsky, Council Chair ALICE-USA Collaboration, in Oxford)
TLC² Outline

• General overview
• Demographics
• Outreach
• External funding
• Infrastructure in support of Research and Education
• Research
TLC$^2$ Mission

to foster and support collaborative multidisciplinary research, education and training in

- Computational Science and Engineering and other disciplines that can benefit from information technology, and in
- Computer Science and Information Technology
TLC² - Current initiatives and centers of excellence

- Abramson Family Center for the Future of Health (joint with the Methodist Hospital Research Institute and Technion-Israel Institute of Technology)
- Advanced Computing Research Laboratory (ACRL)
- Houston Luis Stokes Alliance for Minority Participation (H-LSAMP)
- Institute for Digital Informatics and Analysis (IDIA)
- Institute for Molecular Design (IMD)
- Mission Oriented Seismic Research Program (M-OSRP)
- Southwest Public Safety Technology Center (SWTC)
- Texas Institute for Measurement, Evaluation and Statistics (TIMES)
TLC$^2$ Scope

- Supporting research and education requiring significant computational, storage, networking and visualization resources
  - Provide an infrastructure with significant computing, storage, networking and visualization resources
1.6 TFlops Linux Cluster

- 152 Itanium2 nodes
  - dual 1.3 GHz/3MB processor nodes
  - 4 GB per node
- Myrinet, 152 host ports, 304 spine ports
- GigE for System Area Networking, 4:1 oversubscription
- Management network

- Second most powerful computer in a Texas Educational Institution
- Ranked 102 among the world's 500 most powerful computers (2003)
- Acquired as part of an Intel/HP/TLC² partnership
Distributed Storage Network

Provide NFS based filesystems to SGI, Solaris and Linux clients in Chemistry, Geosciences, Computer Science, and TLC2. RedHat 9.0

2002
2006 ~70 TB

40 TB in eight 5 TB bricks
Dedicated GigE network
SRB

16 TB
30x48TB
HPc 576 - singa1
TLC2 Core Facility

Visualization Laboratory

Clusters

TLC2 Distributed Storage Network

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Visualization Laboratory

SGI Reality Center 3300W
3 Channel Stereo Screen 12.6’ x 23.9’
VHS Video up to 1600 x 1200 @ 60 Hz per channel
3D stereoscopic capability

Immersion Desk R2 4’ x 5’
3D Stereoscopic capability

Visualization Laboratory

Software Packages
• VMD 1.8.2
• OpenInventor 4.0
• Amira 3.1
• MPT 1.9

Compiler Suites
• GCC 3.3
• MIPSpro 7.4

Performance Libraries
• SGI Scientific Library 1.4.1.3

Monitoring/Management Software
• Ganglia Cluster Monitor

On order:
Two Sony 8 Mpixel projectors
Four HP Opteron dual-proc.
dual-core (16 CPU) graphics workstations each with
dual nVidia Quadro FX 4500 video cards
TLC² Computing, Storage and Visualization Facilities

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RENoH – Dark Fiber network

Research
Baylor
MD Anderson
Rice
TAMU HSC
Texas Heart I.
Texas Women U
UTHSC
UH Pharmacy
……

Hospitals
Herman H
Methodist H.
St Luke’s
Shriners
Texas Children’s
………
TLC² Scope

- Supporting research and education requiring significant computational, storage, networking and visualization resources
  - Provide an infrastructure with significant computing, storage, networking and visualization resources
  - State-of-the-art communication tools and electronic classrooms
Classrooms – PGH 200

48 seats with
- 15” flat panel displays
- 1.4 GHz AMD Athlon PCs
- individual teacher – student interaction facilities
Dual boot Linux Windows XP server
AV for video conferencing
Dual projection capability
Streaming video from visualization laboratory

20 – 25 classes/yr
450 – 550 students/yr
Classrooms – PGH 232

126 seats with
Video-conference facilities
Stereographic projection capabilities
Power/Network port at every desk
Communication Facilities

- AG node from InSorS
  - Used regularly for HiPCAT meetings
  - 50% domestic, 50% international

- AV Facilities
  - Video conference capabilities in rooms PGH-200, PGH-218, and PGH-232
  - Ability to direct SGI output to PGH-200, PGH-218 and PGH-232 in addition to displays in PGH-216
  - 10 Keck Center for Computational Biology Seminars Spring 2004
TLC\textsuperscript{2} Scope

- Supporting research and education requiring significant computational, storage, networking and visualization resources
  - Provide an infrastructure with significant computing, storage, networking and visualization resources
  - State-of-the-art communication tools and electronic classrooms
  - Provide expertise in computing and information technology tools development and use (web, data base, HPCN)
TLC\textsuperscript{2} Expertise

- **Data Base expertise**
  - TIMES (supporting awards of $21+ M)
  - H-LSAMP (supporting awards of $8.6M)

- **Web site expertise**
  - About 30 web sites for Labs/Groups, Conferences/Workshops, instruction, developed and maintained (about 10 new sites per year)
  - Quarterly training sessions in web site development and maintenance

- **HPCN expertise**
  - Maintenance of several clusters (about 300 nodes, 100 PCs)
  - Quarterly training courses in cluster configuration and maintenance
  - State-of-the-art (high-performance) networking
TLC² Scope

• Supporting research and education requiring significant computational, storage, networking and visualization resources
  – Provide an infrastructure with significant computing, storage, networking and visualization resources
  – State-of-the-art communication tools and electronic classrooms
  – Provide expertise in computing and information technology tools development and use (web, data base, HPCN)
  – Assistance in proposal preparation and research award management
  – Development of funding opportunities

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## TLC² Proposal activities

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<th>FY2004</th>
<th>FY2005</th>
<th>FY2006 (through July)</th>
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<tr>
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<td>71</td>
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<td>$15.2M</td>
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TLC² Proposal activities

• Colleges
  – Engineering
  – Liberal Arts and Social Sciences
  – Natural Sciences and Mathematics
  – Pharmacy
  – Technology

• Departments
  – Antropology
  – Biology and Biochemistry
  – Chemistry
  – Chemical Engineering
  – Computer Science
  – Economics
  – Geosciences
  – Human Development & Consumer Sciences
  – Mathematics
  – Mechanical Engineering
  – Pharmacy
  – Physics
  – Pharmacological and Pharmaceutical Sciences

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TLC\textsuperscript{2} Scope

- Supporting research and education requiring significant computational, storage, networking and visualization resources
  - Provide an infrastructure with significant computing, storage, networking and visualization resources
  - State-of-the-art communication tools and electronic classrooms
  - Provide expertise in computing and information technology tools development and use (web, database, HPCN)
  - Assistance in proposal preparation and research award management
  - Development of funding opportunities
  - Assistance with arrangements of workshops, symposia, conferences, and external relations
  - Outreach and Promotional efforts (web, flyers, posters, …)
Outreach

- About 10 workshops/Conferences/Symposia per year
- About 10 major local events per year (like hosting/participating in summer camps, high school visits to UH, etc)
- A large number of visits/minor events
- Large numbers of posters
TLC$^2$ Scope

• Supporting research and education requiring significant computational, storage, networking and visualization resources
  – Provide an infrastructure with significant computing, storage, networking and visualization resources
  – State-of-the-art communication tools and electronic classrooms
  – Provide expertise in computing and information technology tools development and use (web, data base, HPCN)
  – Assistance in proposal preparation and research award management
  – Development of funding opportunities
  – Assistance with arrangements of workshops, symposia, conferences, and external relations
  – Outreach and promotional efforts (web, flyers, posters, …)
  – Seed new research initiatives
  – Support innovation in education and training
  – Facilitate the formation of new centers and institutes
TLC² Innovation funding and direct faculty support

<table>
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<th>FY03</th>
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<th>FY05</th>
<th>FY06</th>
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<tr>
<td>$1M</td>
<td>$0.2M</td>
<td>$0.5M</td>
<td>$0.7M</td>
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Examples of TLC$^2$ Research
Mission-Oriented Seismic Research Program

• Research aimed at solving specific highest priority problems

• Problems whose solutions would have the highest positive step-change impact on our ability to find and produce hydrocarbons

• Every link in the seismic processing chain needs to be as effective as the strongest
Seismic Chain

• Acquisition
• Wavelet Estimation
• Multiple Attenuation
• Imaging Primaries
• Inversion of Imaged Primaries
The evolution of science and technology

From less to more complete descriptions of physical phenomena

more realism ⇔ more complete
⇔ more reliable ⇔ less risk

Significant step-change in science requires a vision and methodology that supersedes what came before

Step-change in science (priority) → step-change in prediction

Hence, the alignment!

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We have a record of providing this kind of change:

- **Migration-inversion**, *Stolt and Wegelein* (1985)
- **Wavelet estimation**, *Wegelein and Secrest* (1990)
- **Multiple Removal**, *Wegelein et al.* (1997)
We plan to continue:

• Imaging and inversion at depth without the velocity model (Flagship)

• New methods to determine the wavelet

• Extrapolation and interpolation

• Fundamental new approaches to velocity determination
Mississippi Canyon Free Surface Multiples

Multiples - Water Bottom

Water Bottom Pegleg - Top of Salt

Water bottom

Multiples - Top of Salt

Top of Salt

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Mississippi Canyon Inverse Scattering Multiple Attenuation Example

Brute Stack

Stack after inverse scattering multiple attenuation and deterministic deconvolution

Top of Salt

Base of Salt

Water Bottom Multiples

Water B. Pegleg - Top of Salt

Multiples - Top of Salt

Stack after inverse scattering multiple attenuation and deterministic deconvolution
Internal Multiple Attenuation
Mississippi Canyon Data

Input data
Common offset panel

Estimated
internal multiples

After adaptive
subtraction of multiples

Water Bottom
Top of Salt
Base of Salt
Internal multiple
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<td>Luis Canales</td>
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<tr>
<td>Shell</td>
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<td>Jon Sherman (Chairman, Advisory Board)</td>
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<td>Suresh Thadani</td>
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ALICE in Wonderland

ALICE @ Cern, the Grid
&
UH (TLC² & Physics)

L. Pinsky
CERN in Geneva

- CERN is located in Switzerland & France near Geneva...
- It is the largest particle physics lab in the world...
- The LHC (Large Hadron Collider) project is being constructed NOW...
- ALICE is one of 4 major experiments being deployed at the LHC
- The US has committed ~ $1B already for 2 of the 4 major experiments (ATLAS and CMS
- Major US participation in ALICE is pending at DOE
- UH is a member of ALICE-USA
CERN-LHC & The Grid

• Because of the huge data volumes that are expected to come from the LHC experiments, CERN has been at the forefront of the development of the Grid…

• In the US, the LHC participants have also been a significant driving force in Grid Development…

• UH has been a player in this game, and is getting increasingly involved…
ALICE @ CERN

- ALICE (A Large Ion Collider Experiment) One of the Major Experiments @ the LHC Project
- CERN (World’s Largest Particle Physics Research Center in Geneva, Switzerland)
- >1000 Physicists from 83 Institutions in 27 Countries
- ALICE-USA Currently consists of 16 US Institutions
- L. Pinsky (UH) is the Computing Coordinator for ALICE-USA…

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The ALICE Data Challenge

- ALICE will produce ~1.7 PB/Year of Raw Data, and an annual net storage requirement for > 4.0 PB/Year...
- The Reduction of that data will require the commitment of ~16,000 kSI2k of CPU...
- In the US, we will need >400 TB/year of storage and 3,400 kSI2k of CPU...
- Note that TLC²’s fastest Itanium nodes are <1kSI2k...
- …And all of this data needs to be moved around easily and quickly!

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The Grid…

• The Grid is more than just a method of distributing computing remotely…
  – It allows seamless:
    • Distribution of programs and files…Access to run on available resources anywhere…(Where “Resources” can be soft or hard…)
    • Collaboration at a Distance…

• To Function well, a Grid needs BANDWIDTH as well as Computing Power and Storage…

• UH is now a member of PPDG, one of the major US DOE-sponsored Grid development Projects, and we are establishing contacts with iVGDL and GriPhyN, two other major US Grid Projects… Being part of ALICE gives us particular leverage due to the most recent developments!
The “Political” Situation

- There is likely to be ~$4M for ALICE hardware in the US from DoE and NSF…

- Our “Collaborators” include Ohio State (and the Ohio Supercomputing Center), and NERSC at LBNL (UC Berkeley).

- OSC is highly leveraged by the State of Ohio, and NERSC is a DoE favorite “son.”

- To be in a position to be a player, we need:
  - An ability to leverage our purchasing like Ohio, and…
  - Have access via a competitive bandwidth…
Life Sciences
What is Different in our Approach

Counting Arrays

Algorithms for the problem of finding appearances of all possible patterns of size $n$ in a sequence

*Prucheslav Pofinov*, *Varty Pofinov*, *E.* and *B. Montgomery Pettit*1,2

1Department of Computer Science University of Houston, Houston, Texas
2Department of Chemistry University of Houston, Houston, Texas

We can do it extremely fast for up to 25-mers
We create new approaches to identify locations of pathogenic islands in genome using statistical properties.
Case Study: Botulism Toxin

• Botulism toxins are the most poisonous substances known!

• Iraq generated 19,000 liters of concentrated toxin and loaded half of it into missiles – much of the toxin was never found.

• One teaspoon of botulism toxin can kill ONE MILLION people!

• However, 3.5 nanograms (3.5x10^-9) of BoTox can be used to temporarily eliminate facial wrinkles.

Searching for new drugs

- Molecular flexibility is taken into account
- Databases contain millions of molecules
- Computations done at TLC$^2$: 6.4 CPU years

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Molecular Dynamics Simulations

- **raw trajectory**
  - solute
  - solvent
  - 10^4 - 10^7 timesteps
  - 10^3 - 10^6 particles

- **processed data**
  - 10^1 - 10^7 values
  - 1 - 10^3 quantities

- **analysis**

- **final processing**

- **final output**

- **time and memory**
  - 0.1 - 100 GB
  - 10^2 - 10^5 CPU seconds
  - 1 - 1000 MB
  - 10^1 - 10^2 CPU seconds
  - 1 - 1000 KB

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MD simulations and Grids
EM Imaging

No. of Particles Needed for 3-D Reconstruction

<table>
<thead>
<tr>
<th>Resolution</th>
<th>B = 100 Å²</th>
<th>B = 50 Å²</th>
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<td>8.5 Å</td>
<td>6,000</td>
<td>3,000</td>
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<tr>
<td>4.5 Å</td>
<td>5,000,000</td>
<td>150,000</td>
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</table>

8.5 Å Structure of the HSV-1 Capsid
EM imaging

EMAN Database
- Archival
- Data Mining
- Management

Vitrification Robot

EMAN
- Initial 3D Model
- Reproject 3D Model
- Build New 3D Model
- Align Average Deconvolute
- Classify Particles
- Particle Selection Power Spectrum Analysis

Micrographs
- 4 - 64 Mpxels, 16-bit (8 – 128 MB)
- 100 – 200/day per lab
- 10 – 1,000 particles per micrograph
- Several TB/yr

Project
- 200 – 10,000+ micrographs
- 10,000 – 10,000,00 particles
- 10k – 1,000k pixels/particle
- Up to hundreds of PFlops

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VGrADS Virtual Grid Application Development Software

Carl Kesselman
Keith Cooper
Ken Kennedy
Charles Koelbel
Richard Tapia
Linda Torczon

Rich Wolski
Fran Berman
Andrew Chien
Henri Casanova

Lennart Johnsson

Plus many graduate students, postdocs, and technical staff!

An NSF-funded Information Technology Research project

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VGrADS Application Collaborations

**EMAN**
Electron Micrograph Analysis

**GridSAT**
Boolean Satisfiability

**LEAD**
Atmospheric Science

**Montage**
Astronomy

**Data**
arrives

**Resource**
Broker

**Dynamic**
Workflow

**Static**
Workflow

**BPEL** Workflow Engine

**LDM** Service

**GridFTP Service**

**WRF** Service

**Ensemble Broker**

**Data Mining**

**Information Service**

**Rice Scheduler**

**Visualization Service**

**vgES**

**SAT problem:**

Decision stack before conflict:
- Level 6: \( V_1 \)
- Level 4: \( \neg V_1 \)
- Level 3: \( V_2 \)
- Level 1: \( V_3 \)

Decision stack after backtracking:
- Level 4: \( \neg V_1 \)
- Level 2: \( V_2 \)
- Level 1: \( V_3 \)
- Level 0: \( V_4 \)

Learned clause: \( -V_3 + V_4 + V_5 - V_6 \)

**Figure 1:** Examples of conflict analysis with learning and non-chronological backtracking.

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Research at UT-IDIA

Institute for Digital Informatics and Analysis

Research focus: fundamental problems with a universal range of applications

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I. Pixel-processing without tears: Directionally unbiased multi-dimensional signal processing

- Fast isotropic wavelet decomposition (prototype complete, refined versions in developmental stage)
- Frame-based wavelet multi-resolution analysis (patent submitted)
- Use of DAF Sparkle™ technology
Application:
Cardiology (first prototype software (fps) completed)

MicroCT slices
before

after filtering.

slices through coronary

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Application:

Mammography (patent claims approved; fps completed; work in progress with group at M. D. Anderson)

Isotropic deconvolution with DAF Sparkle™ technology

before

after

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National Digital Mammography Archive

- About 40 million mammograms/yr (USA) (estimates 32 – 48 million)
- About 250,000 new breast cancer cases detected each year
- Over 10,000 units (analogue)
- Image size: 4kx6k, about 48 MB
- Images per patient: 4
- Data set size per patient: about 200 Mbytes
- Data set per year: about 10 Pbytes
- Data set per unit, if digital: 1 Tbytes/yr, on average
Early Bilinguals
SN/ED

Right

Left

Spanish more active
English more active

(Hernandez, A.E., Dapretto, M., Mazziotta, J. & Bookheimer, S., 2001)

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Proteomics


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Collaboration

SuperHD Streaming Video

100-Megapixel Tiled Display

Augmented Reality

The ENDFusion Project
A High Definition Access Grid as Imagined In 2007 In A HiPerCollab

Source: Jason Leigh, EVL, UIC
## Summary: Bandwidth Needs

<table>
<thead>
<tr>
<th>Discipline</th>
<th>Size of Archives</th>
<th>Growth rate of Archives</th>
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<tbody>
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<td>Life Sciences</td>
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<tr>
<td>Mammography</td>
<td>50 – 100 PB</td>
<td>25 – 60 PB/yr</td>
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<tr>
<td>Microscopy</td>
<td>100+ PB</td>
<td>50 – 100 PB/yr</td>
<td>1 – 10 Gbps</td>
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<tr>
<td>Other imaging</td>
<td>200+ PB</td>
<td>100+ PB/yr</td>
<td>10 – 100 Gbps</td>
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<td>Major medical center</td>
<td>100 – 1,000PB</td>
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<td>~100 Gbps</td>
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<td>Earth Sciences</td>
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<td>Weather</td>
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<td>1 – 10 Gbps</td>
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<tr>
<td>Climate</td>
<td>100+ PB</td>
<td>50 – 100 PB/yr</td>
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<tr>
<td>Environment</td>
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<tr>
<td>High-Energy Physics</td>
<td>100+ PB</td>
<td>20 – 50 PB/yr</td>
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<td>Telemedicine, Telescience</td>
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<td>Computation</td>
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Summary

Research and Education needs high capacity networks, and for real-time collaboration low latency, low jitter networks.