

STATE UNIVERSITY AT BUFFALO



# HPC<sup>NY</sup>

UB CCR's Industry Cluster  
*Center for Computational Research*








# What is HPC<sup>NY</sup>?

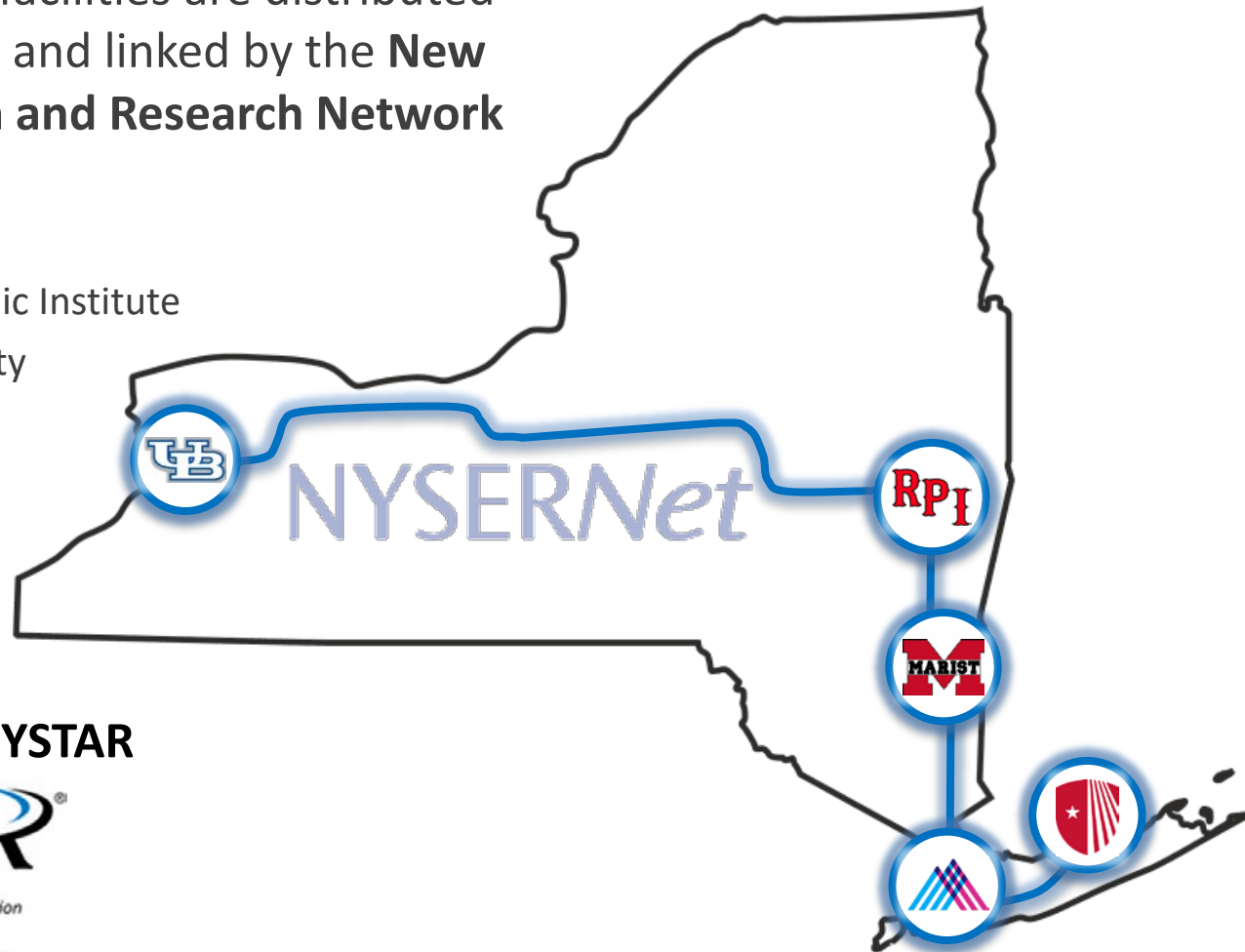
- HPC<sup>NY</sup> is New York State's **High Performance Computing Consortium**.
- A network of university computing centers who partner with industries throughout the state to help foster business growth and process improvement.
- An HPC<sup>NY</sup> partnership can help companies **create jobs, save costs, accelerate R&D, and obtain funding**.
- HPC<sup>NY</sup> provides access to computational resources and world class expertise in **modeling, visualization, and analytics**.
- Funded by ESD/NYSTAR.



# HPC<sup>NY</sup> : Computational and intellectual breadth

- HPC<sup>NY</sup> expertise and facilities are distributed throughout the state and linked by the **New York State Education and Research Network (NYSERNet)**:

-  University at Buffalo
-  Rensselaer Polytechnic Institute
-  Stony Brook University
-  Marist College
-  Mount Sinai



Powered by ESD/NYSTAR



# The UB CCR industry cluster

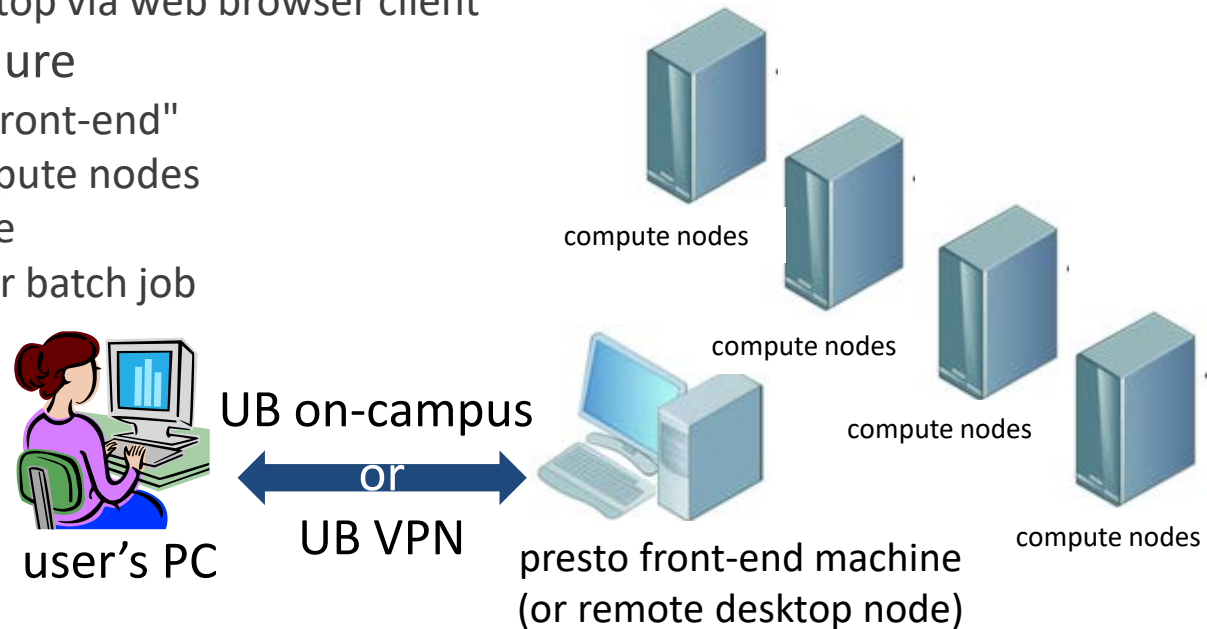
- \$1.2 Million supercomputer
- 3456 processors
- 72 TFLOPS peak performance
- Faculty and staff expertise:
  - genomics, bioinformatics
  - computer vision, comp. science
  - engineering, CFD, GIS
  - molecular modeling
  - computational chemistry
  - crystallography, volcanology
  - many other areas!



Industry Cluster Node Rack

# Cluster Access

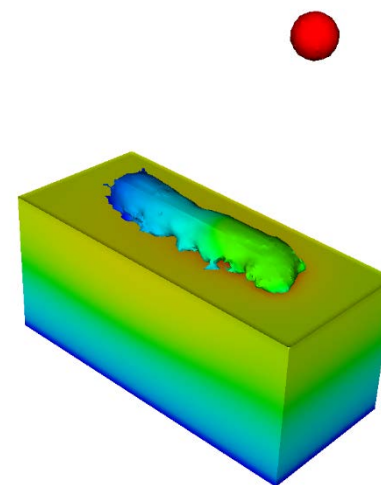
- Secure remote access
  - Hardware and software firewalls
  - Virtual Private Network
  - Secure Shell
- Two modes of access:
  - Linux command line via xterm and ssh
  - Remote desktop via web browser client
- General Procedure
  - Connect to "front-end"
  - Request compute nodes
  - Load software
  - Launch GUI or batch job



## Example Partner: VADER Systems

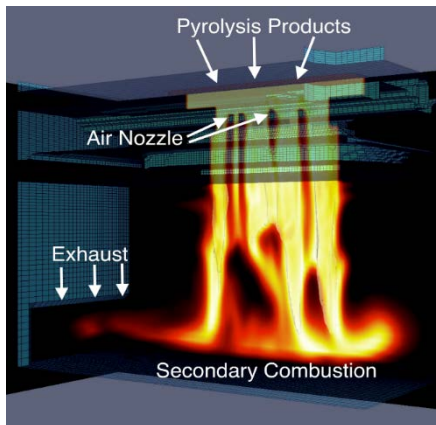
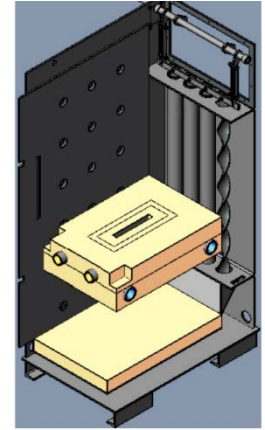
- Additive manufacturing using Liquid Metal Jet Printing (LMJP)
  - layered droplets of molten metal
- Use UB CCR to simulate droplet generation and engineer droplet behavior while cooling on the substrate
- The partnership accelerated their MK1 product launch
  - In time for rollout of the RIT AMPrint (Additive Manufacturing and Multifunctional Printing) Center
- Now looking at new materials and running at higher temperatures and faster printing rates

VADER



## Example Partner: Econoburn Inc.

- Econoburn designs and manufactures 2-stage boilers in Brocton, NY
- Partnered with UB and UB CCR to maximize burn efficiency and minimize emissions
- Assisted by faculty from Department of Mechanical and Aerospace Engineering
  - Experts in CFD and turbulent flow



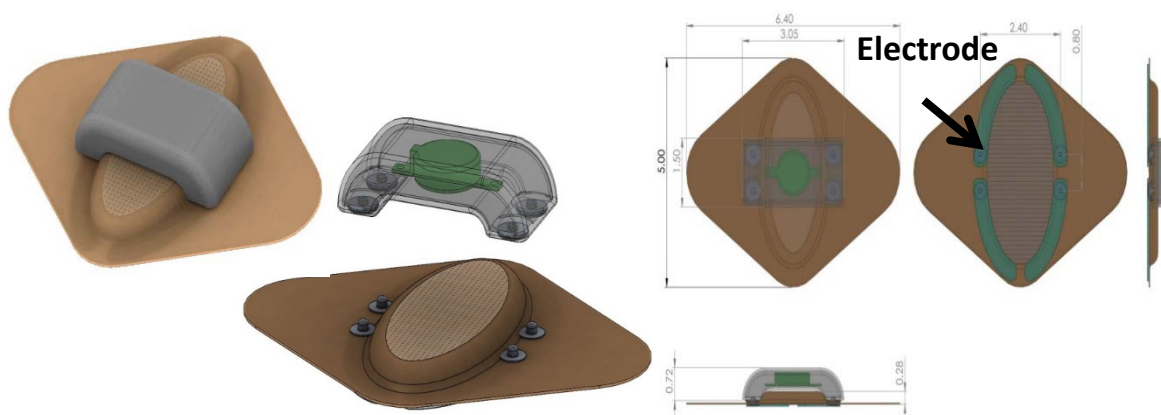
- Understanding turbulent flow at extreme temperatures is key to the success of the technology
  - **A common problem in many manufacturing environments, where materials must be rapidly heated and/or cooled**
- Flow simulations carried out on CCR industry cluster and then verified on physical prototype

## Example Partner: Garwood Medical

- “Smart Bandages” for patient-specific wound healing
- Remotely powered and equipped with wireless sensors to collect biometrics and monitor compliance
- Electrostimulation prevents infections associated with surgical implants
- Product development is being accelerated through the use of HPC resources to model complex interactions between human tissue, implants, bacteria, and electrochemistry



GARWOOD MEDICAL  
DEVICES, LLC





## Example Partner: Sentient Science Inc.

- Sentient's DigitalClone software runs at UB CCR
  - Predicts failure in rotating assets (turbines, blades, etc.)
- Currently contracted to monitor 62,500 wind turbines in the field to improve operational efficiency
- **30+ new high tech jobs created in Buffalo since 2013 and another 70+ expected by 2018**
  - \$10 Million in sales in 2016
  - expecting \$20 Million in sales in 2017
- **“Quite simply, there is no way that we could sustain this growth without access to UB CCR's resources and computing expertise.”** --- *Ward Thomas, CEO*



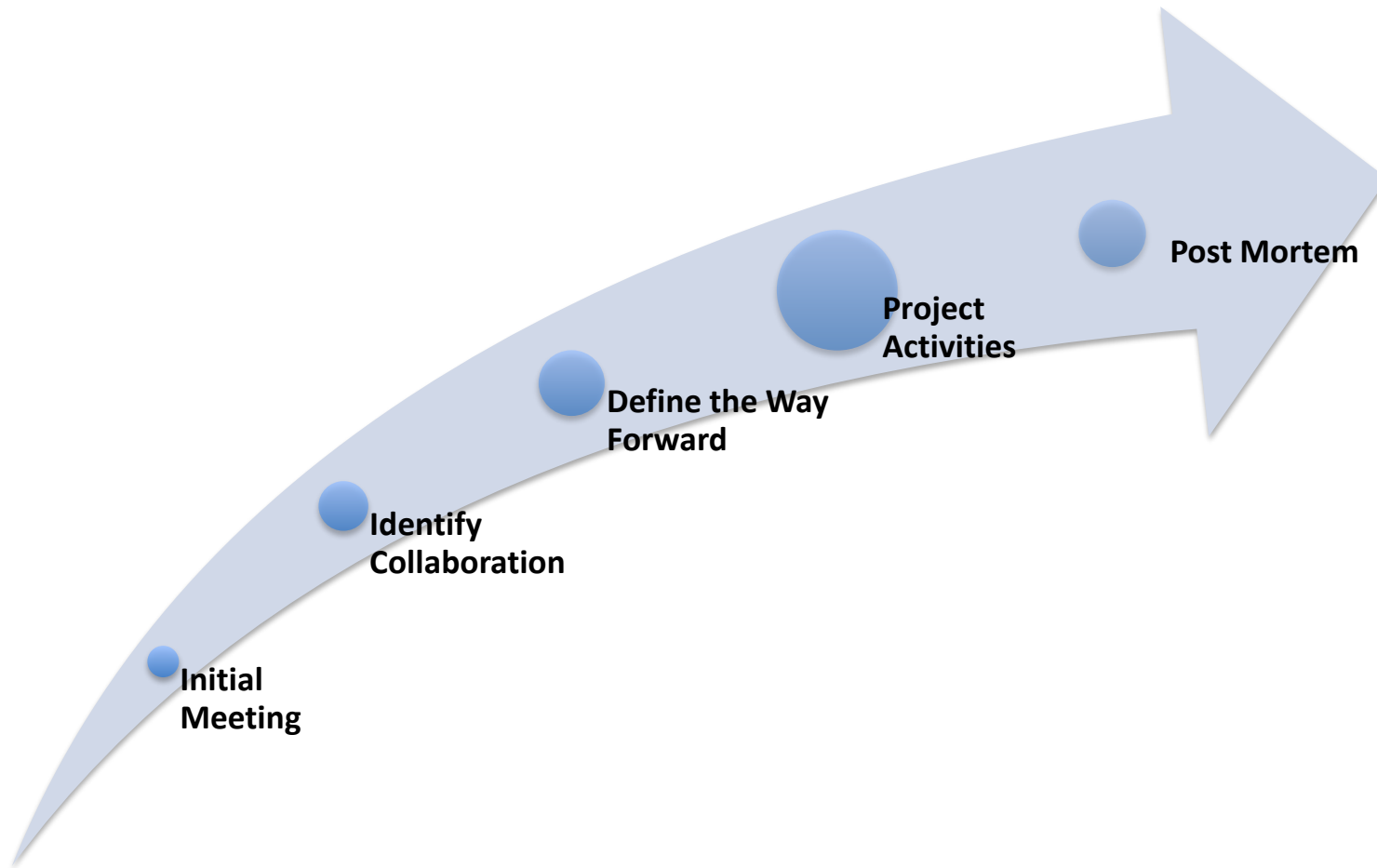
# Is HPC<sup>NY</sup> Right for Your Company?

- Does your company use any computational or scientific software (e.g. COMSOL, ANSYS, MATLAB, etc.)?
- Is controlling or understanding heating/cooling/flow important to your company's day-to-day operations?
- Does your company have any internal R&D staff or does your staff perform custom engineering?
- Is your company able to dedicate staff (or funding) a short-term project?
- Has your company competed (or is interested in competing) for federal or state grants (e.g. NSF, NIH, DOE, SBIR/STTR, NYS CAT, etc.)?

## Some areas where HPC<sup>NY</sup> can help your company ...

- Computational or scientific software
- Heating/cooling/flow operations
- Internal R&D problems
- Custom engineering
- External grant funding and support letters
- Faculty expertise and connections
- Automated drug discovery
- Informatics processing pipelines
- Machine/deep learning and artificial intelligence
- Big Data and analytics
- Image and pattern recognition
- High-speed rendering
- Database engineering

# Overview of UB CCR Collaboration Workflow



# Where to go for more information

- Contact CCR
  - Dr. Tom Furlani, Director, [furlani@buffalo.edu](mailto:furlani@buffalo.edu), 716-881-8939
- Contact a UB CCR HPC<sup>NY</sup> outreach coordinator:



Dr. Shawn Matott  
Computational Scientist  
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716-881-7566

Adrian Levesque, MBA  
Project Manager  
[apl3@buffalo.edu](mailto:apl3@buffalo.edu)  
716-881-8932



- Explore the CCR Web Site - [www.buffalo.edu/ccr](http://www.buffalo.edu/ccr)
- Explore the HPC<sup>NY</sup> Web Site - [www.hpc-ny.org](http://www.hpc-ny.org)
- Contact HPC<sup>NY</sup>
  - Edward Reinfurt, Business Development Officer  
518-573-3537 (cell), 518-276-6699 (office), [reinfe@rpi.edu](mailto:reinfe@rpi.edu)

# Software Modules

Engineering	Machine Learning	Hadoop/MapReduce	Math/Physics	Image Processing	Utilities
ABAQUS	Caffe	Hadoop	BandUP	EMAN2	7zip
ANSYS	Caffe2	HBase	CrystFEL	FFMPEG	Ant
AVL FIRE	Keras	Hive	FEniCS	OpenCV	CMAKE
CFX	MikeNet	Pig	GAP	OpenEXR	DMTCP
COMSOL	TensorFlow	Spark	Gnuid	OpenSlide	gnu-parallel
CPLEX	Theano	ZooKeeper	Gurobi	<b>Environmental</b>	HDF/HDF5
DAKOTA	Torch	<b>GPU Programming</b>	kmos	Cantera	KchmViewer
iso2mesh	<b>Data Analytics</b>	CUDA	ROOT	GRASS	lxml
LSDYNA	edgar	Intel-OpenCL	VMTK	HYSPLIT	Mono
NETGEN	Jags	OpenCL	<b>Visualization</b>	LANDIS-II	netCDF, NCO, CDO
OpenFOAM	MCL	PyCUDA	de.caff	MODFLOW	pbzip2
OpenSees	ms	<b>Editors</b>	NCL	NaSt3DGP	pigz
pyFormex	R	Emacs	ParaView	puffin	TauBench
QUCS	SAS	Idle	TecPlot	TELEMAC	tmux
SALOME	Stan	NetBeans	VTK	TITAN	xclip
StarCCM	STATA	Vim	xmgrace	WRF-WPS	xfig

# More Software Modules

Molecular Dynamics	Quantum Chemistry	Libraries (cont.)	Programming	Programming (cont.)
Amber , AmberTools	ABINIT	Elemental	Cilk	Julia
AutoDock	Dalton	GLPK	DDT/MAP	Mathematica
CHARMM	Elk	GMP	DMD	MATLAB
CP2k	GAMESS	Intel: MKL, MPI, TBB	gcc , gdb	Maven
GROMACS	GPAW	libgd	golang	Mercurial
LAMMPS	NWChem	libgpuarray	google-api	mpiP
MDAnalysis	OpenBabel	libgtextutils	IDL	Octave
MMTSB	Orca	libmatheval	Intel-Advisor	PAPI
MODELLER	Q-Chem	libmesh	Intel-CLCK	Perl
NAMD	QUANTUM ESPRESSO	mvapich2	Intel-Compiler	PGI
OpenMM	Siesta	OpenBLAS	Intel-DAAL	PP (Parallel Python)
PLUMED	<b>Libraries</b>	OpenMPI	Intel-Inspector	Python
pyRosetta , Rosetta	Armadillo	PETSc , SLEPc	Intel-IPP	Rdesktop
Schrodinger	ARPACK	scikit-tensor	Intel-ITAC	Scala
supercell	BOOST	TetGen	Intel-vTune	SCons
VMD	CGAL	Tioga	Java	Valgrind

# Even More Software Modules!

Bioinformatics / Genomics (130 modules)									
AdmixTools	BedTools	CNVnator	fusioncatcher	Kallisto	miRDeep2	PARE	qctool	seqtk	TopHat
Admixture	bio3d	Cromwell	gatk	Kraken	MixMapper	PATSER	QIIME	Snpeff	Tracer
AlignGraph	bioconda	Cufflinks	GCTA	lobSTR	mothur	pBlat	Randfold	Snpsift	TreeMix
AML	bioperl	cutadapt	genipe	lumpy-sv	MrBayes	picard	RAXML	Snptest	TrimGalore
ANGSD	BLASR	DADI	GMAP	MACS	MSMC	Pindel	RELION	SomaticSniper	Trinity
ANNOVAR	BLAST	deepTools	GTOOL	MACS2	MuMmer	PLINK	RSem	speedseq	VarDict
BadiRate	Blat	deFuse	HLAreporter	mapDamage	NCBI	PLINK/SEQ	RSeQC	Squid	VCFtools
Bambino	Bowtie	dice	HOMER	MEME	NgsAdmix	Polysolver	Sailfish	SRA Toolkit	VEGAS2 / VEGAS2v02
bam-readcount	Bowtie2	EIGENSOFT	HTSeq	MERLIN	ngsPopGen	Preplot	Salmon	Strelka	Velvet
BamTools	BreakDancer	EMBOSS	HTSlib	METAL	NgsRelate	Preseq	SAMtools	StringTie	VEP
bcl2fastq	BWA	EPACTS	IgBLAST	MetAMOS	nucleo	ProDy	schmutzi	SurvivalGWAS_SV	ViennaRNA
Beagle	CDK	FastQC	Jellyfish	Minimac3	OpenGATE	psmc	SeqAn	svtyper	WDLtool
BEAST2	CGHub	FASTX	JointSNVMix	MIRA	PAML	PyBedTools	SEQLinkage	tabix	XWAS