# INDUSTRY CLUSTER USAGE

May 2019

## 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

## Industry Cluster Expansion

- $1 Million Expansion
- Focusing on GPU Architecture
- Supports:
  - Artificial Intelligence
  - Machine Learning
  - Blockchain
- Available for usage late 2019/early 2020

# 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

# Cluster Access (cont.)

user's PC

UB on-campus

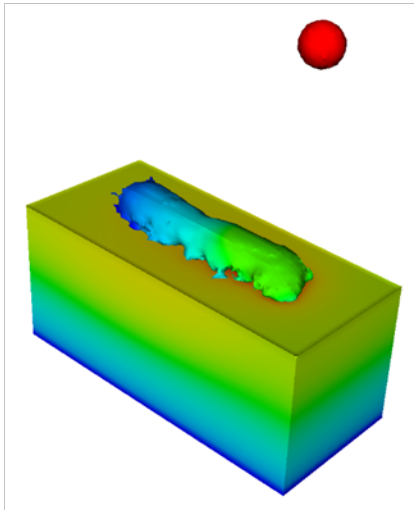
UB VPN

presto front-end machine
(or remote desktop node)

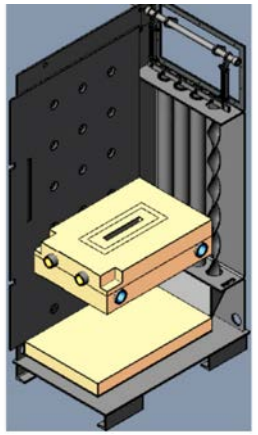
# Example Partner: VADER Systems

- 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
- Purchased by Xerox in Feb 2019

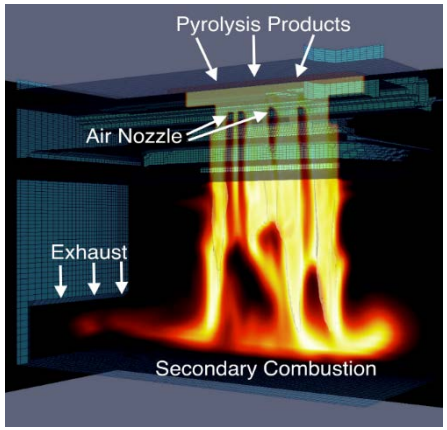
VADER



# Example Partner: Econoburn Inc.



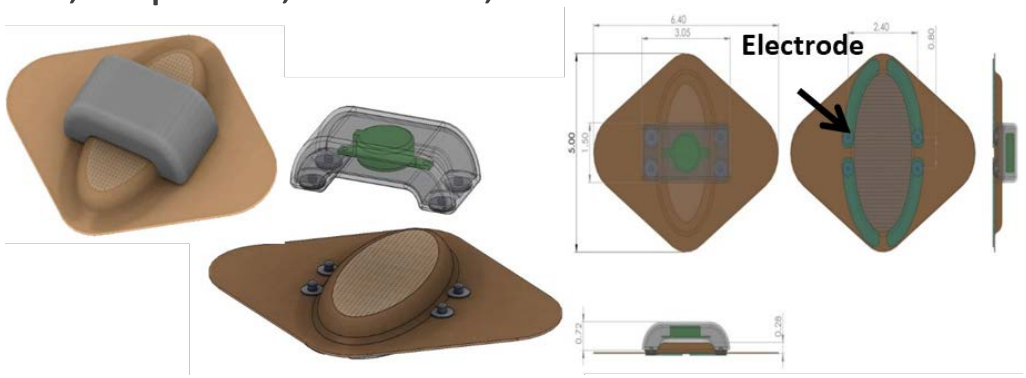
- Econoburn designs and manufactures 2-stage boilers in Brocton, NY
- Partnered with UB and UB CCR to maximize burn efficiency and minimize emissions
- Assisted by faculty from Department of Mechanical and Aerospace Engineering
  - Experts in CFD and turbulent flow
- Understanding turbulent flow at extreme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


- Use materials science to build computational models of complex rotating machines, such as wind turbines.
- Winner of numerous national awards in Energy
- Currently monitor over 40,000 Wind Turbines in the field to improve operational efficiency (10% of turbines worldwide)
- Sentient's DigitalClone software runs at UB's Center for Computational Research to provide a prognostic life forecast of major systems and components in the wind, aerospace and transportation to achieve lower operations and maintenance costs.
- 80 jobs created/retained to date

# Is CCR's Industry Cluster Right for Your Company?

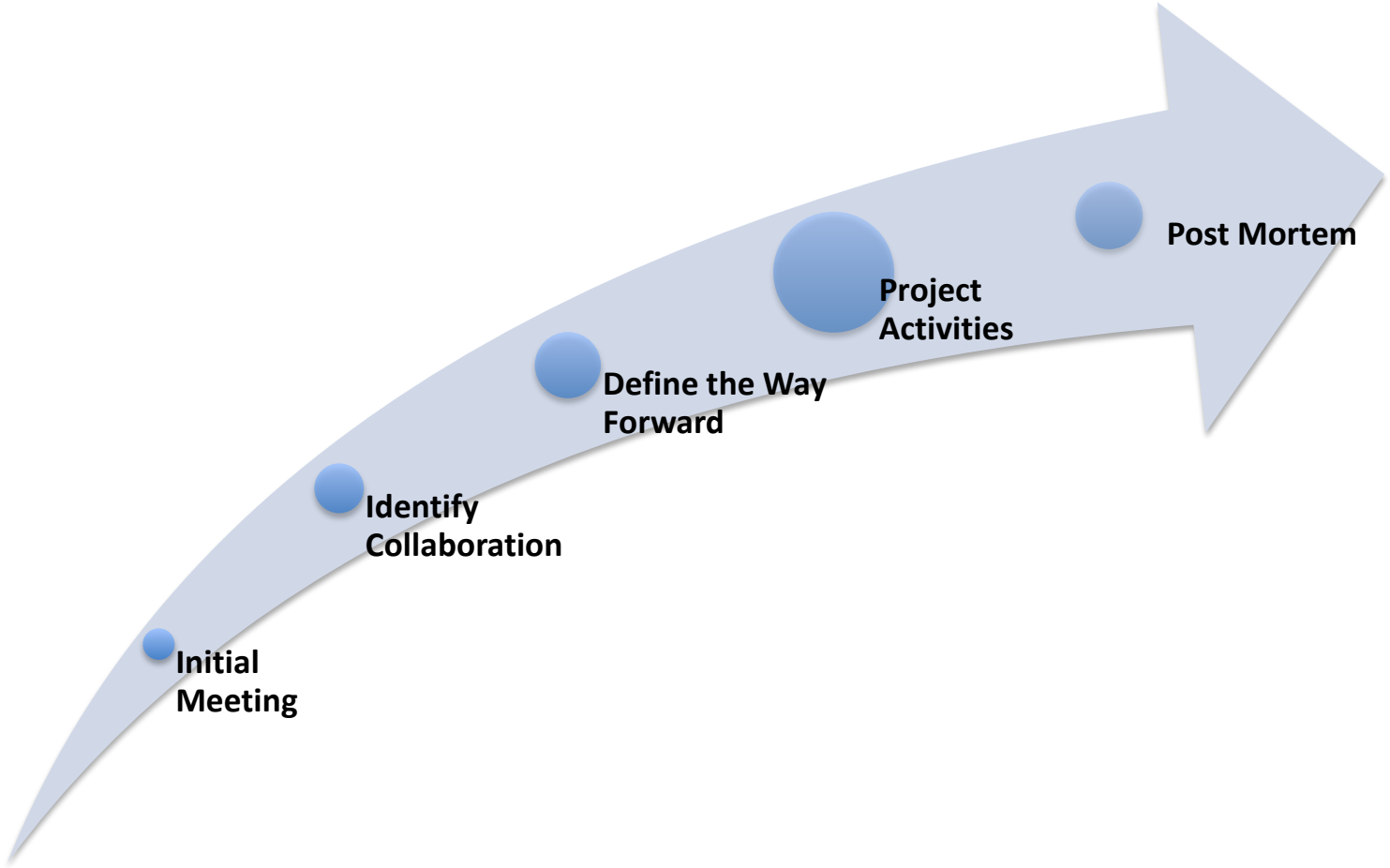
- Does your company use any computational or scientific software (e.g. COMSOL, ANSYS, MATLAB, etc.)?
- Is controlling or understanding heating/cooling/flow important to your company's day-to-day operations?
- Does your company have any internal R&D staff or does your staff perform custom engineering?
- 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 CCR may be able to help…

- 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

*Hardware support coming late 2019 / early 2020

# Overview of CCR Industry Collaboration Workflow



# Where to go for more information

- Contact a UB CCR Industry Outreach lead:

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- Explore the CCR Web Site - www.buffalo.edu/ccr

# 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 | **Environmental** | HDF/HDF5 |
| DAKOTA | Torch | **GPU Programming** | kmos | Cantera | KchmViewer |
| iso2mesh | **Data Analytics** | CUDA | ROOT | GRASS | lxml |
| LSDYNA | edgar | Intel-OpenCL | VMTK | HYSPLIT | Mono |
| NETGEN | Jags | OpenCL | **Visualization** | LANDIS-II | netCDF, NCO, CDO |
| OpenFOAM | MCL | PyCUDA | de.caff | MODFLOW | pbzip2 |
| OpenSees | ms | **Editors** | 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 |

# Software Modules (cont.)

| 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 | Libraries | 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 |

# Software Modules (cont.)

| 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 |