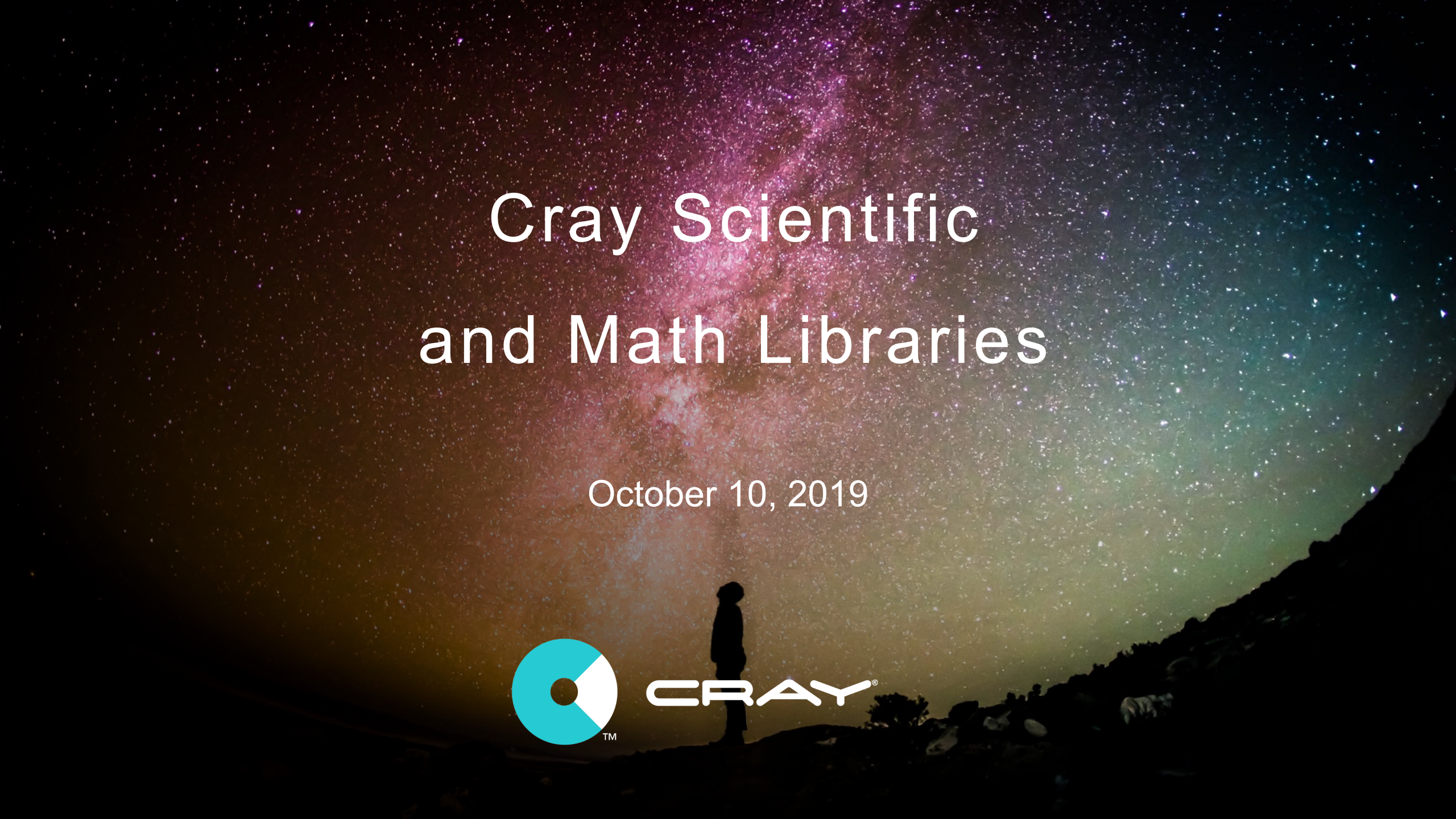
Cray Scientific
and Math Libraries
October 10, 2019
CRAY

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Cray Scientific and Math Libraries (CSML)

- CSML releases a wide range of libraries useful for a variety of different scientific applications
  - Examples of scientific applications that make use of CSML libraries:
    - CP2K, LSMS, Qbox, Quantum ESPRESSO
    - Other applications in areas of computational fluid flow, multiphysics, and climate

- Include linear algebra routines for matrix operations, factorization, solvers, FFT

- Optimizations focus on dense linear algebra routines for CPU and GPU targets

What Do Cray Scientific Libraries Offer?

- **Designed to achieve maximum performance from Cray systems with minimum effort**

- **Node performance**
  - Highly tuned BLAS within nodes

- **Network performance**
  - Optimized for performance across nodes
  - Overlap between communication and computation
  - Use the best available low-level mechanism
  - Use adaptive parallel algorithms

- **Highly adaptive software**
  - Using auto-tuning and adaptation, provide the best known algorithms at runtime

- **Productivity features**
  - Simpler interfaces into complex software

Core Libraries Available Today

- Accessible by loading modules
  - cray-libsci
    - CPU targeted optimized BLAS, LAPACK, ScaLAPACK, IRT
  - cray-libsci_acc
    - GPU targeted optimized subset of BLAS, LAPACK, ScaLAPACK
  - cray-fftw
    - CPU targeted optimized FFTW package

Using CSML

- Current CPUs and GPUs supported include Intel Xeon, AMD EPYC, Nvidia GPUs

- Available today on Cray XC systems and works with
  - CCE, GNU, and Intel compilers
  - cray-mpich

- Available today on Cray CS systems and works with
  - CCE compiler
  - cray-mvapich2 and Intel MPI

- Libraries are automatically included at link time by Cray cc, CC, and ftn drivers when modulefile is loaded

Overview of cray-libsci

- Optimized set of BLAS, LAPACK, and ScaLAPACK libraries
  - Optimized for Intel Xeon (AVX-512) and AMD EPYC (AVX2) CPU targets
- Package includes Iterative Refinement Toolkit (IRT) set of linear solvers
  - Uses IR with mixed-precision to accelerate LU and Cholesky solvers
- Optional eigenvalue solver ScaLAPACK backends available:
  - KAUST KSVD with ZOLO-PD - optimized for large ill-conditioned inputs
  - ELPA – symmetric eigensolver (must provide path to an external self-built ELPA package)
- Cray libraries are integrated into cray-python and cray-R packages
  - NumPy and SciPy packages in cray-python leverage cray-libsci for matrix ops

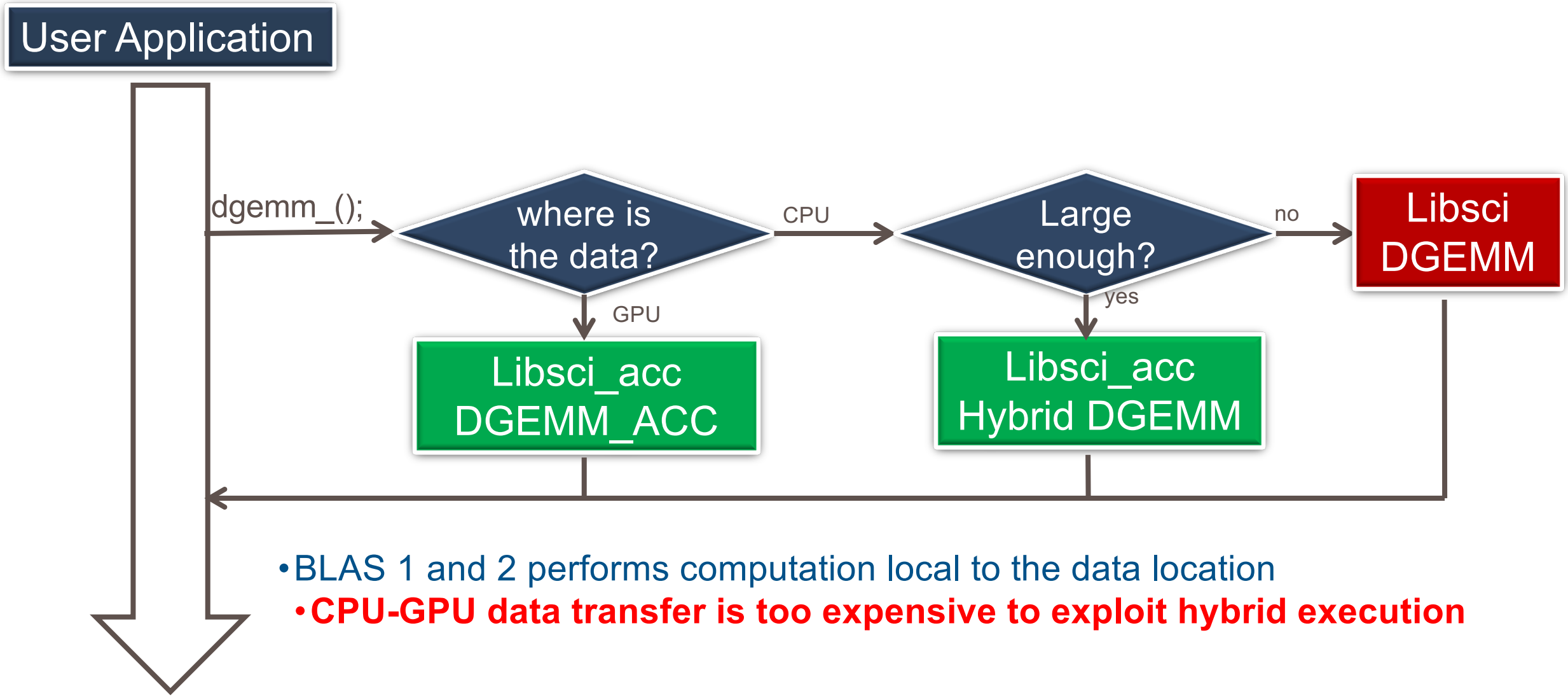
Overview of cray-libsci_acc

- Provides basic scientific libraries optimized for hybrid systems
  - Includes a subset of GPU optimized BLAS, LAPACK, and ScaLAPACK routines
- Independent to, but fully compatible with OpenMP
- Intended primarily as a drop-in for CPU codes to port them to GPU targets
  - For example a CPU dgemm_(tA, tB, M, …) call in code would be off-loaded
- Currently support Nvidia Tesla GPGPU targets including Pascal and Volta
  - Support for AMD GPUs coming next year

Using cray-libsci_acc

- To use, make sure the following module is loaded:
  - `user@login> module load cray-libsci_acc`
  - Automatically loaded if GPU target module set, for example craype-accel-nvidia60
- Automatic and manual cray-libsci_acc interfaces
  - Automatic interface will detect and orchestrate CPU-GPU memory transfers
    - Includes out-of-core support (example: matrix multiple is blocked to avoid GPU memory overflow)
  - Manual interface is explicit about where memory is allocated
    - May be useful for finer control
- Currently supports OpenACC and OpenMP offload
- See intro_libsci_acc man page for more details

Automatic Interface for BLAS3 and LAPACK



- BLAS 1 and 2 performs computation local to the data location
  - **CPU-GPU data transfer is too expensive to exploit hybrid execution**

Overview of cray-fftw

- Cray optimized version of the popular FFTW library
- Includes serial, threaded, and distributed (via MPI) FFTW libraries
- Supports C2C, R2C, C2R, and R2R FFTs of arbitrary size and Ndims
- Tuned for Intel Xeon (AVX-512) and AMD EPYC (AVX-2) targets
  - Includes optimized plan data for typical inputs for scientific applications
- Supports a variety of in-place and out-of-place FFT operations

Using cray-fftw

- FFTW3 libraries automatically included via Cray `cc, CC, ftn` drivers
  - `user@login> module load cray-fftw`
- Independent to, but fully compatible with OpenMP
- Uses the standard FFTW3 interfaces and API
- See intro_fftw3 man page for more details

Thank You!

QUESTIONS?