CyberGIS Toolkit: A Software Toolbox Built for Scalable cyberGIS Spatial Analysis and Modeling

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Outline

- Purposes
- Software integration approach
  - Software component selection
  - Software engineering
  - Scalability analysis
- Progress update
  - CyberGIS Toolkit 0.5-alpha release
  - Continuous integration framework
  - Deployment on advanced cyberinfrastructure
- Case study: Parallel PySAL (pPySAL)
  - Parallel PySAL project
  - Illustration of parallelization strategies
- Future work and concluding discussion

Six Major Goals of the NSF CyberGIS Project

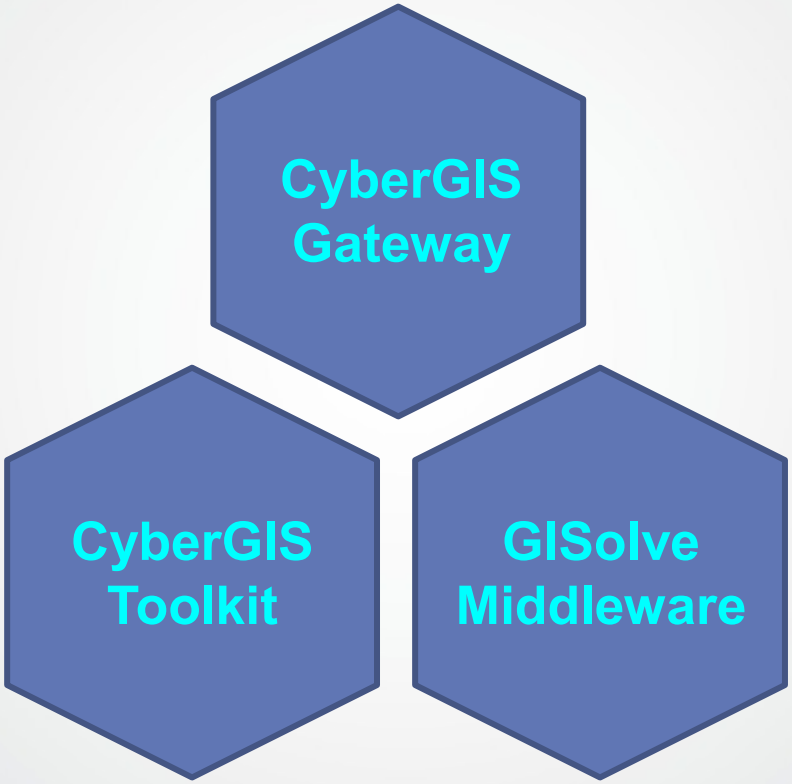
1. Enga communities through a participatory approach to re requirements;
2. Integrate and sustain a core set of composable, interoperable, manageable, and reusable CyberGIS software elements based on community-driven and open source strategies;
3. Empower high-performance and scalable CyberGIS by exploiting spatial characteristics of data and analytical operations for achieving unprecedented capabilities for geospatial scientific discoveries;
4. Enha patial problem solving environment to allow for the contr learning of CyberGIS software by numerous users e development of crosscutting education, outreach and training programs with significant broad impacts;
5. Deploy and test CyberGIS software by linking with national and international cyberinfrastructure to achieve scalability to significant sizes of geospatial problems, amounts of cyberinfrastructure resources, and numbers of users; and
6. Evalu e CyberGIS framework through domain science appli partnerships to gain better understanding of the comp man-natural systems.

Software as deliverables

Building blocks

Computational solutions

CyberGIS Software Environment



"CyberGIS Toolkit, a deep approach to CyberGIS software integration research and development, is focused on developing and leveraging innovative computational strategies needed to solve significant geospatial scientific problems by exploiting high-end cyberinfrastructure (CI) resources."

-- NSF CyberGIS Project, 3rd Year Annual Report (2013)

Objectives

- Identify and integrate a set of loosely coupled scalable geospatial software components into the CyberGIS Toolkit
- Establish and sustain the CyberGIS Toolkit as a reliable software toolbox through an open and rigorous software building, testing, packaging, and deployment framework
- Capture computational and spatial characteristics of a software element focusing on computational performance, scalability, and portability in various CI environments
  - XSEDE (Extreme Science and Engineering Discovery Environment. http://xsede.org)
  - Open Science Grid
  - Extreme-scale supercomputers
- Provide a software environment for computational and data scientists to easily configure and use CyberGIS Toolkit components

Software Integration Approach

- Software component selection
  - Open source strategy
  - Community-driven component identification
    - Benefits to related science areas
- Software engineering
  - Complexity in software integration
  - A holistic framework for streamlined component integration
- CI-based scalability evaluation and enhancement
  - Computational intensity analysis – theoretical approach
  - Performance analysis and profiling – experimental approach

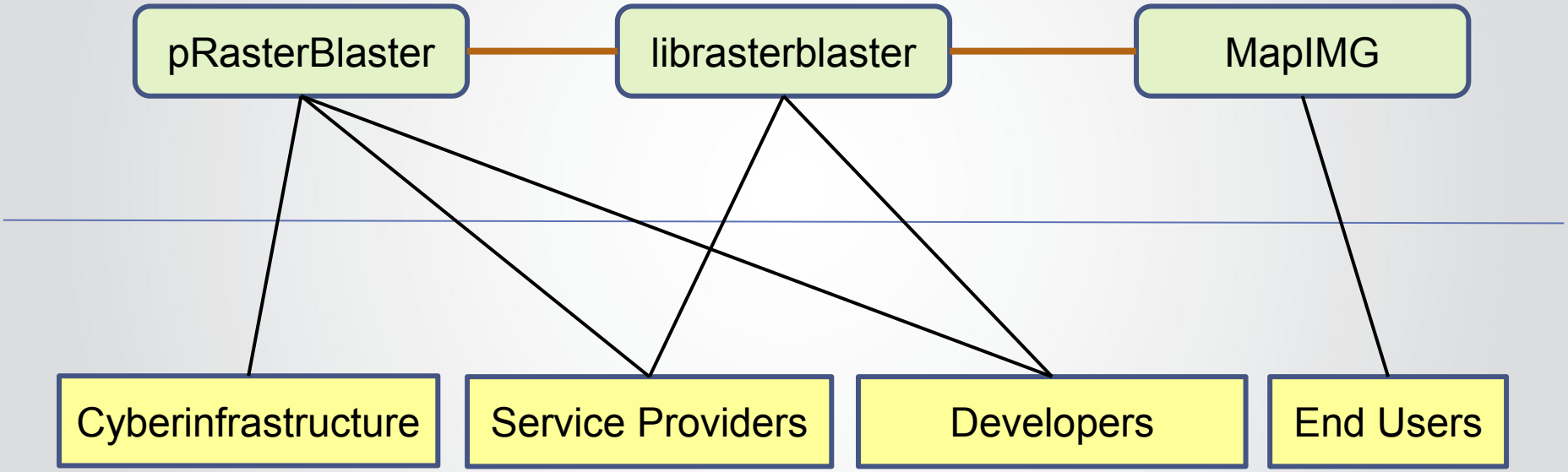
Open Source Strategy

- Components
  - Each component must be open sourced
  - No restriction on any particular open source license
- Toolkit
  - Improves the accessibility to integrated software capabilities through the establishment of a software toolbox
  - Focuses on the robustness, portability, compatibility, and scalability of each component within advanced CI environments

Component Selection Example: pRasterBlaster

- Need for scalable map reprojection in cyberGIS analytics
  - Spatial analysis and modeling
    - Distance calculation on raster cells requires appropriate projection
  - Visualization
    - Reprojection for faster visualization on Web Mercator base maps
- pRasterBlaster integration in CyberGIS Toolkit and Gateway
  - Software componentization: librasterblaster, pRasterBlaster, MapIMG
  - Build, test, and documentation
  - Gateway user interface

pRasterBlaster Component View



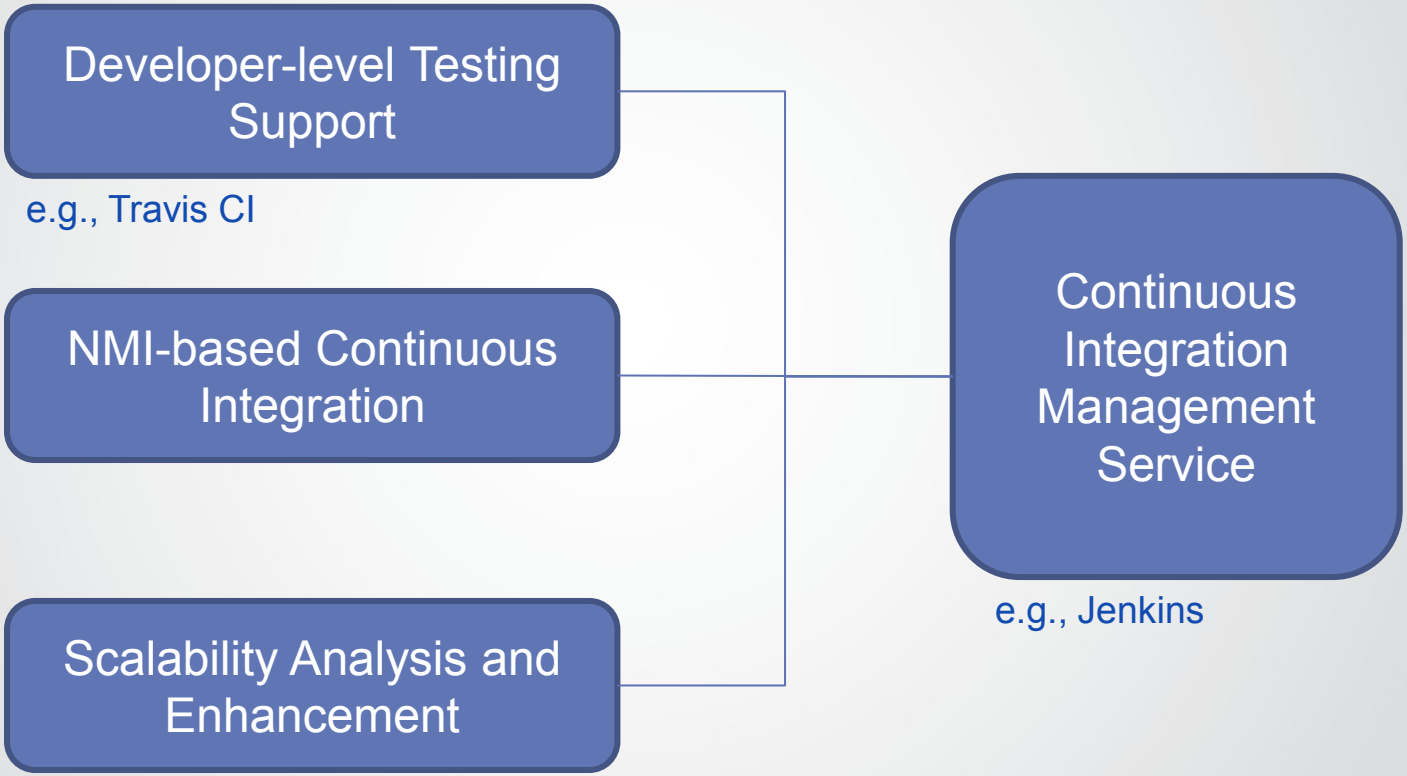
Integration Challenges

- Diversity and heterogeneity of software components
  - Programming languages
  - Application *vs.* library
  - Dependent libraries
  - Code availability
  - Programming models
  - Cyberinfrastructure resources
- Multiple levels of integration
  - Desktop level
  - Heterogeneous software environments
  - Cyberinfrastructure
- Software distribution
  - CI deployment
  - Packaging for broader distribution

Strategies

- Build and test
  - Establish a streamlined process to build and test software codes
- Computational intensity analysis
  - Computational bottleneck evaluation
  - Scalability analysis
  - Generalize solutions as computational and spatial knowledge
- Packaging and distribution
  - Package software for download and build in user computing environments
  - Provide common distribution packages (Debian, RPM, Windows installer, etc.)
  - Establish CyberGIS Toolkit as a configurable software module that can be loaded/unloaded on supercomputers
- Documentation and training
  - Build a CyberGIS Toolkit web site to host the software suite, user guide , development documentation, education materials, user feedbacks, and forums
  - Develop online training materials

Continuous Integration Framework



NMI: National Middleware Initiative (http://batlab.org)

Component Integration Process

- Selection
- Parallelization
- Development of test cases
- Development of build and test plans
- NMI regular build and test
- Scalability analysis on CI
  - Identification of potential computational bottlenecks
  - Scalability to the number of processors
  - Scalability to problem size
- Release in the CyberGIS Toolkit
- Accessibility in CyberGIS
  - Cyberinfrastructure deployment for high-end users
  - Lowering access barriers for community users through Gateway and GISolve
  - Incorporation in advanced application workflow

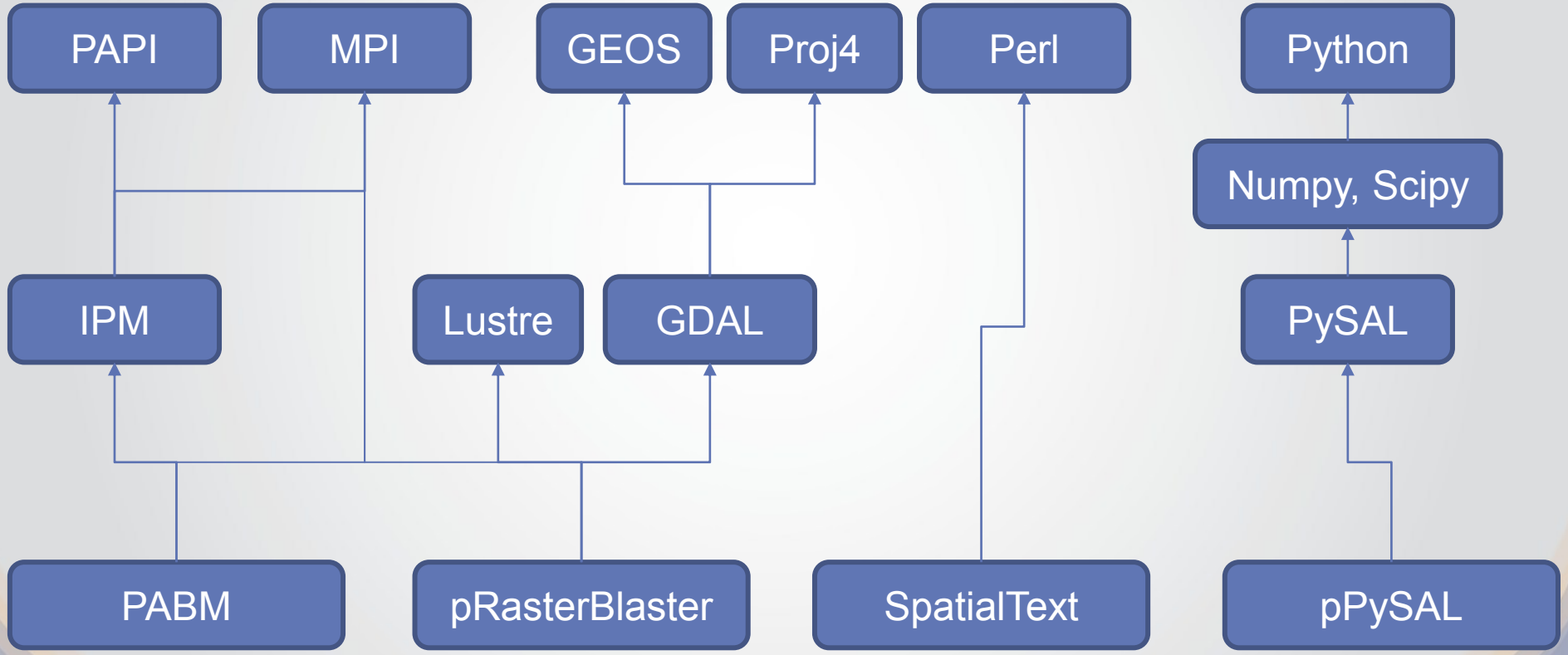
Demo

- CyberGIS Toolkit 0.5-alpha release
  - http://cybergis.cigi.uiuc.edu/cyberGISwiki/doku.php/ct

Software Components

- Parallel Agent-Based Modeling – PABM
  - HPC models: MPI, parallel I/O
  - Contributor: UIUC team
- Parallel PySAL
  - Parallel python implementation
  - Contributor: ASU team
- Parallel map reprojection – pRasterBlaster
  - HPC models: MPI, parallel I/O
  - Contributor: High-performance mapping group, CEGIS, USGS
- SpatialText
  - Full-text geocoding of massive social media and text data
  - Contributor: Kalev Leetaru and UIUC team

Dependency Graph – CyberGIS Toolkit 0.5-alpha



Toolkit Deployment on XSEDE

- XSEDE resources
  - Stampede@TACC: 10 petaflops; cluster computing, multi-threaded, GPU computing
  - Lonestar@TACC: 0.3 petaflops; cluster computing, multi-threaded, large memory
  - Trestles@SDSC: 0.1 petaflops; cluster computing, data I/O intensive computing
  - Gordon@SDSC: 0.34 petaflops; cluster computing, data I/O intensive computing, large memory
  - Blacklight@PSC: 0.037 petaflops; shared memory
  - Keeneland@NICS: cluster computing, GPU computing
- Compiling and install
  - Compilers: Intel, GNU, PGI
  - MPI: Open MPI, mvapich2, mpich2, PGI, Intel MPI
- Software environment configuration
  - Environment Modules
  - Adaptive software module loading/unloading
  - Demo

Case Study: Parallel PySAL

Serge Rey, Jay Laura

Concluding Discussion

- The first set of selected software components has been integrated into the CyberGIS Toolkit 0.5-alpha
- A prototype integration framework has been established to allow sophisticated multi-level integration tests
- Scalability analysis has been effective to identify computational bottlenecks and improve the performance of several components
- CyberGIS Toolkit has been deployed on XSEDE for community access
  - Through GISolve Open Service API
- Community evaluation and feedback is critical for building high-quality and scientifically sound software

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We need your feedback!

Contact: dev@cybergis.org

Thanks!