Software for USNDP

Michael Smith
Physics Division
Oak Ridge National Lab
Oak Ridge, Tennessee
Motivation

- Strong need for **new software tools** was repeatedly expressed by researchers at the Notre Dame Workshop
  - opportunity for researchers to more fully utilize USNDP products
  - many creative ideas, but lack expertise to implement and resources to maintain

Software for USNDP

Michael Smith
• **Strong need for new software tools** has also been requested by SOME evaluators
  
  – opportunity for evaluators to benefit from recent software innovations to increase productivity, accuracy, reliability ...
  
  – some new tools are being developed (JAVA NDS)
  
  – IAEA has moved in this direction (MyENSDF, X4 tools ...)

**Software for USNDP**

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### Categories of Software

<table>
<thead>
<tr>
<th></th>
<th>Visualization</th>
<th>Data Diving</th>
<th>Workflow</th>
<th>Executable</th>
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<tr>
<td><strong>Access Codes</strong></td>
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<td><strong>Science Codes</strong></td>
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<td><strong>and Pipelines</strong></td>
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<td><strong>Evaluator Tools</strong></td>
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- Many different types of software used in nuclear science
- Matrix of code categories suggests gains from parallel development of multiple tools by reusing code components
“Software business as usual” will not meet community requests for new tools or realize possible gains in productivity, ease-of-use …

- Software has a lower priority than evaluation work
- Software development requires different skill set
- Any proposal for incremental software work within the USNDP will compete for funds with evaluations

Significant progress will require a new approach
• Suggested Key Features

− finite performance period (such as 3 years)
− focus on projects rated highest priority
− realistic milestones and deliverables
− well managed effort with project controls
− separate funding
− not replace / conflict with ongoing work
− involve professional level coders advised by data experts
• Things to do
  – query Users for projects
  – prioritize projects
  – query Users for features / preferences
  – pay attention to interfaces (storyboards)
  – emphasize pipelining when possible
  – include heavy documentation
  – provide multiple views / paths / approaches
  – provide in-system help / guides / manuals
  – provide upgrade paths
• Things to avoid … don’t
  – develop tools that aren’t needed
  – duplicate efforts
  – focus on new formats (too controversial)
  – work with proprietary architectures
  – assume all Users want the same features
  – keep codes proprietary
More things to avoid ... don’t
- build for a single platform
- exclusively use old paradigms (downloads)
- ignore cloud-based solutions
- develop in a vacuum (ignore other products)
- assume others will develop tools we request
- assume that one solution will work for all
Computational Infrastructure for Nuclear Astrophysics
- Cloud-based solution offering unique capabilities in the field that span the range from nuclear data to reaction rates to simulations
- Enables users to upload, manipulate, manage, visualize, share nuclear information and complex simulations

Nuclear Mass Toolkit
- Cloud-based solution offering unique comparisons between mass data sets from evaluations, compilations, experiments, and theory

Big Bang Nucleosynthesis
- Users can set up and run custom simulations of element creation in the early universe

Cloud Computing
- Plenary talk at ND2010 on Cloud Computing for Nuclear Data envisioned a new paradigm for data activities
- NDC3.net established to host future work

Bellerophon*
- Huge expansion of CINA for supernova simulations on ORNL Supercomputers

BEAM*
- Expansion of Bellerophon for materials science research at ORNL, spanning desktops, clusters, supercomputers with drag-and-drop queueing and file transfers

* Led by Eric Lingerfelt
• Isotopes.gov
  – Modernized DOE’s isotope program IT infrastructure
  – Cloud solution features catalog with multiple entry methods, ordering, preferred customers “one click” ordering features, top-notch security, tool kit and interface custom designed for Isotope Business Office, custom permissions, associated expansive website …
  – Time-saving “snapshots” of data activities can do a weeks work with a few clicks … duplicates functions of excel, powerpoint, pdf exports
  – Done as separate DOE Project with milestones & project controls
Path Forward

• identify sponsors
• gather interested parties
• discuss possible projects
• solicit project suggestions from community
• prioritize projects
• write and submit proposal