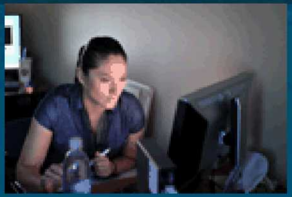
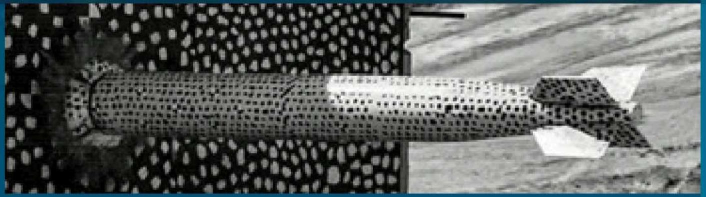
SAND2018-14134PE

NEXT GENERATION SEVERE ACCIDENT AND DYNAMIC EVENT TREE MODELING





PRESENTED BY

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Team Member Acknowledgements

- MELCOR3
  - Randall Gauntt: Project Management, Severe Accident Expert
  - Larry Humphries: MELCOR2 Lead Developer, Severe Accident Modeling Expert
  - Vince Mousseau: MELCOR3 Lead Developer, Physics Expert (RELAP5, TRAC, TRACE)
  - Aaron Krueger: MELCOR3 Numerics, MEA, MMS, MEAMMS
  - (I am MELCOR3's Software Architect and SQA Lead)
- ADAPT
  - Zac Jankovsky: ADAPT Lead Developer, Dynamic Event Tree Expert
  - Matt Denman: Project Management, PRA Expert, Big Picture Design
  - (I aid ADAPT in development of tools, APIs, and website interface design)

Motivation

- Next generation severe accident modelling needs to
  - model a multitude of materials, interactions, closures, components, systems, etc.
  - explore the numerous permutations of postulated events, actions, and their consequences
  - provide quantitative insights for many different quantities of interest

Study Every Pebble, Walk Every Path, Limit No Horizon

"It's your study, you can do whatever you want. Then you'll get criticized for it."

— Michael Corradini,
ACRS Regulatory Policies and
Practices Subcommittee Meeting,
October 18, 2017

Outline

- MELCOR3 (physics simulator)
  - MELCOR2
  - Advancing State-of-the-Art
  - Design and Features
    - Core Principles
    - Foundational Features
    - Our Quality Process
    - Significant Uncertainty Minimization ("whack-a-mole")
    - Summary and Future
- ADAPT (dynamic event tree driver)
  - Purpose
  - History
  - Design and Features
  - Applications
  - Summary and Future

MELCOR3

MELCOR2

- Overview
  - A fully integrated, engineering-level computer code that models the progression of severe accidents in light-water reactor nuclear power plants
  - Objective
    - Consistent modelling of relevant phenomena for source term calculation
    - Recent expanded scope includes containment response, advanced reactor analysis, and more
  - Absolute top in its class
- Physics models
  - Decay heat loading and initial fission product distribution
  - Corium formation, relocation, and concrete interaction
  - Radionuclide release, transport, deposition, resuspension
  - Hydrogen deflagrations and containment response
  - Thermohydraulic response given initial coolant loading and external injections
  - And much more…

Advancing State-of-the-Art

- Why MELCOR3?
  - MELCOR2 models are extensive and well-exercised.
  - Architecture is primary target: more flexible, more extensible, several levels of fidelity
- Generalization of the conservation framework
  - Current
    - 4-field for thermohydraulics
    - 12-field for core degradation (29-field if radionuclides are included)
    - A few solution algorithms implemented directly in-code
  - Advancement
    - n-field for all materials
    - everything is a moveable and fail-able
    - A generic problem structure that is reduced to an optimal, per-situation solution algorithm.
- Move toward a plug-in architecture
  - Current: separation based on physics bundled with solvers, explicit coupling
  - Advancement: separation of solvers, closures, numerics, fluxes, sources, and facilities for global coupling
- Other Points
  - General residual-based framework
  - Automatic verification of transport equations
  - Incorporate knowledge and needed structure of modern analysis techniques from the beginning
  - And more…

There is a lot to unpack here!
Let's get more specific.

Design and Features

- Core Principles
- Foundational Features
- Our Quality Process
- Significant Uncertainty Minimization ("whack-a-mole")

Each of these is a talk on their own. To follow: a broad, dense overview.

Disclaimer: MELCOR3 is a work-in-progress, and details presented here may change in the future.

Core Principles (1/4)

- Don't assume; measure and assess.
- There are an arbitrary number of fields (water, air, fuel, steel, etc.).
  - Solver shall not care nor need knowledge of field information beyond residual value
- Every field shall evolve such that (Constraints keep solution on a "surface of realizability")
  1. mass is conserved,
  2. energy is conserved,
  3. momentum is conserved,
  4. entropy is increased,
  5. all physics have length scales and time scales.

Core Principles (2/4)

- How many types of equations are currently considered by MELCOR3?
- Scalar Conservation (for k-th field)

$$V\frac{\phi_k^{n+1}-\phi_k^n}{\Delta t}-\left(\sum_{\text{in}}\text{flux}_{\text{in}}(\phi_k)-\sum_{\text{out}}\text{flux}_{\text{out}}(\phi_k)+\sum\text{sources}_k\right)=0$$

- Vector Conservation (for k-th field)

$$V\frac{(\rho u)_k^{n+1}-(\rho u)_k^n}{\Delta t}-\left(\sum_{\text{faces}}\text{forces}_k+\sum\text{sources}_k\right)=0$$

- Linearization (for k-th value)

$$q_k=q_k^*+\frac{\partial q_k}{\partial q_m}(q_k^*-q_m^*)+\frac{\partial^2 q_k}{\partial q_l\partial q_m}\frac{(q_k^*-q_m^*)(q_k^*-q_l^*)}{2}+\text{H.O.T.}$$

Core Principles (3/4)

- The fields evolve with the discrete, control volume equations
  - All fluxes, forces, and sources must be conservative/telescoping (conservation)
  - All fluxes, forces, and sources must lead to an increase in entropy
- Every term in the equations (all fluxes, forces, sources, and time differences) will be individually tracked and analyzed
  - Local truncation error is measured and ensured small
  - Length scales are estimated and resolved through meshing
  - Time scales are estimated and resolved time step adjustment

Core Principles (4/4)

- Solution Method
  - Jacobian-Free
  - Consistent Physics-based Preconditioning (Preconditioner converges to Jacobian upon iteration)
  - Linear (Krylov) Solver: Preconditioned Generalized Minimal Residual (PGMRES)
- Newton's Method

$$\frac{\partial r(q^k)}{\partial q^k}\,\delta q^k = -r(q^k)\left[-\frac{\partial^2 r(q^k)}{\partial {q^k}^2}\frac{\delta q^k \delta q^k}{2} + \text{H.O.T.}\right]$$

- Jacobian "Action" Approximation

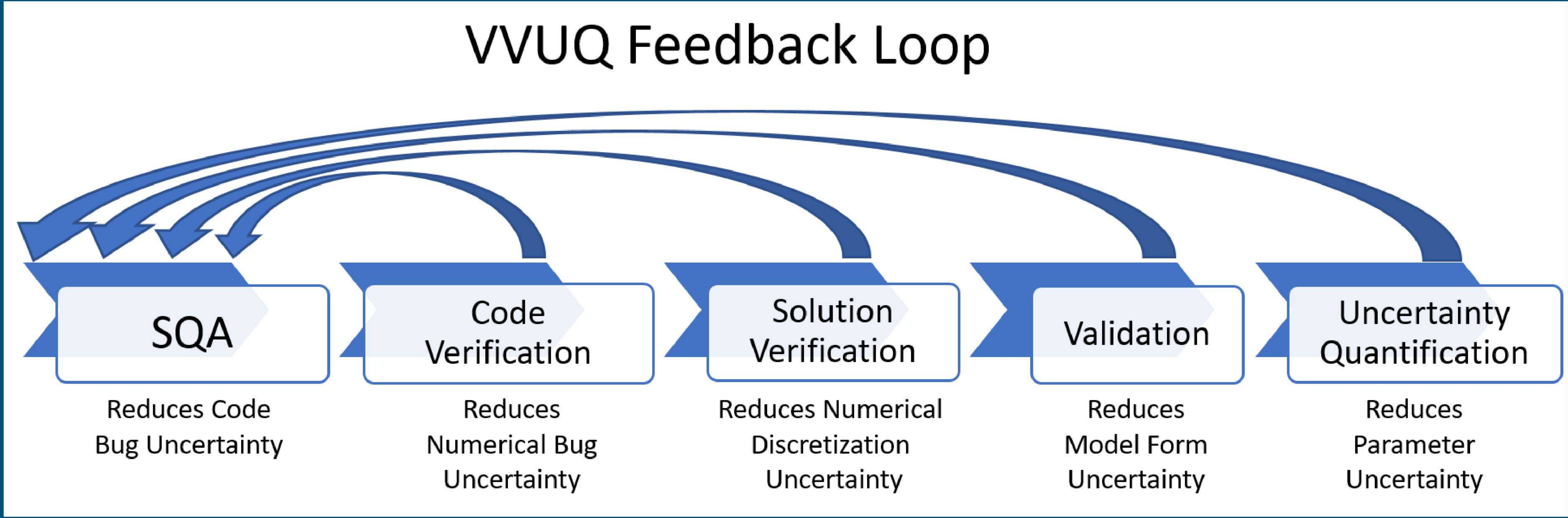
$$\frac{\partial r(q^k)}{\partial q^k}\,\delta q^k \approx \frac{r(q^k + \varepsilon\,\delta q^k) - r(q^k)}{\varepsilon}\left[-\,\varepsilon\,\frac{\partial^2 r(q^k)}{\partial {q^k}^2}\frac{\delta q^k \delta q^k}{2} + \text{H.O.T.}\right]$$

Foundational Features

- MELCOR3 parlance: Matryoshkas
- Physics Matryoshka:
  - Ability to merge fields (i.e., create a HEM) arbitrarily with a measure of efficacy
  - Example:
    - Two fields: liquid water and steam
    - Can simulate separately with burden of boiling/condensation time scales
    - Can also HEM together with a set of difference equations monitoring “distance” from HEM
- Geometry Matryoshka
  - Just like Physics Matryoshka: ability to join control volumes together with a measure of efficacy
- Solver Matryoshka
  - Similar to above: explicit, semi-implicit, fully implicit depending on time scales and lengths
- Spatial Error and Temporal Error Monitoring
  - Use previous quadratic terms and H.O.T. to measure errors
  - Change control volume size, time step size to keep small (“drive the bus”)

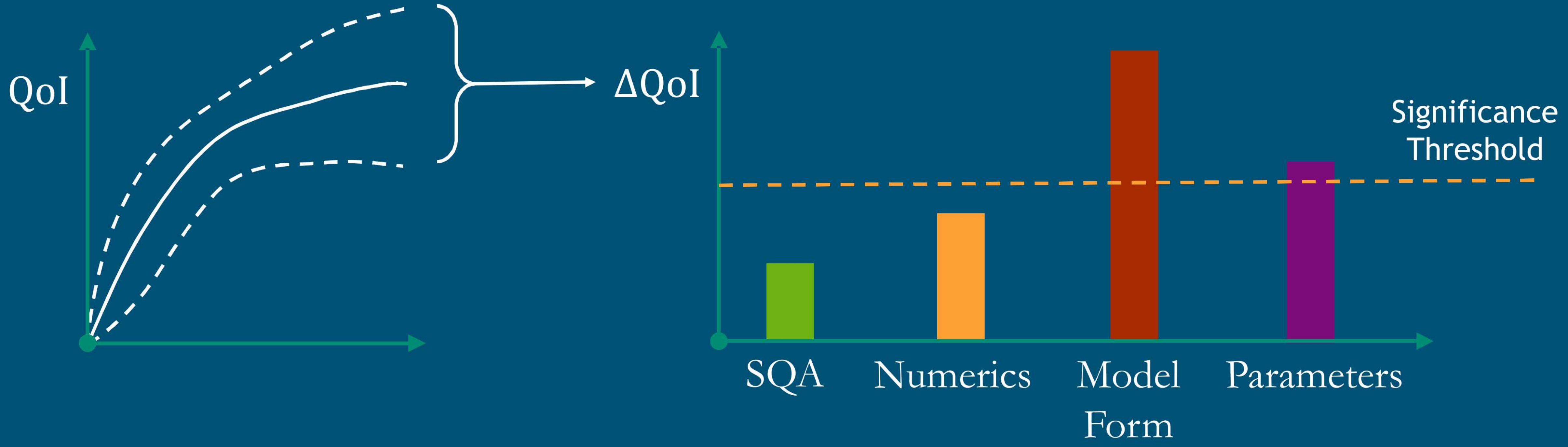
Our Quality Process

- Matryoshkas, Spatial Error, Temporal error allow quantification of
  - Numerical error
  - Model Form error (different models; e.g., interfacial friction)
  - Parameter uncertainty (same model; e.g., exponents in Dittus-Boelter)



Significant Uncertainty Minimization ("whack-a-mole")

- Fictitious example for a given Quantity of Interest (QoI)



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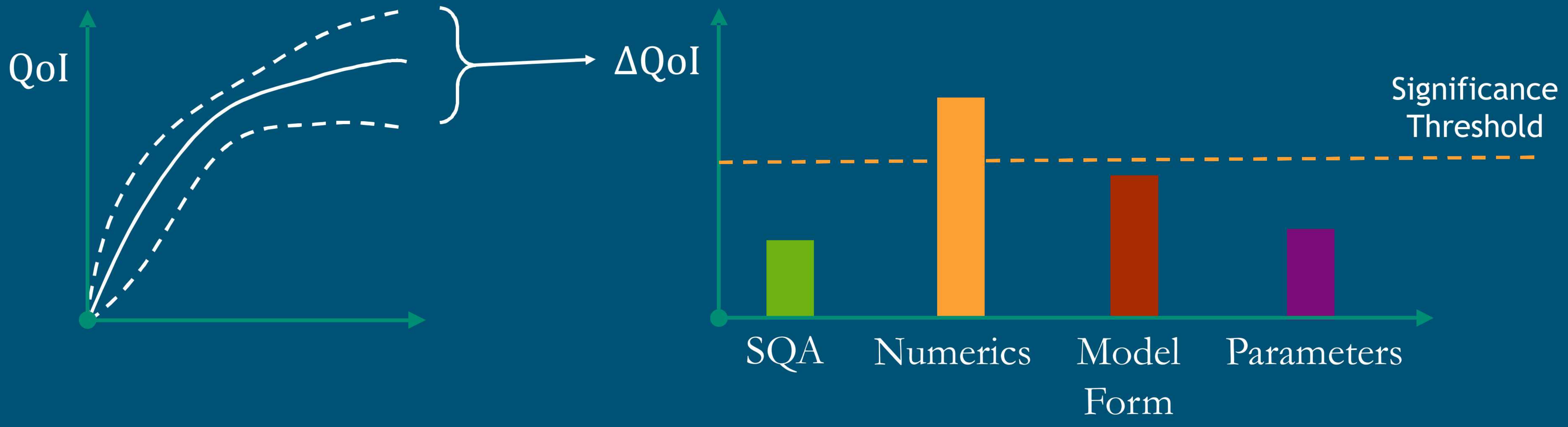

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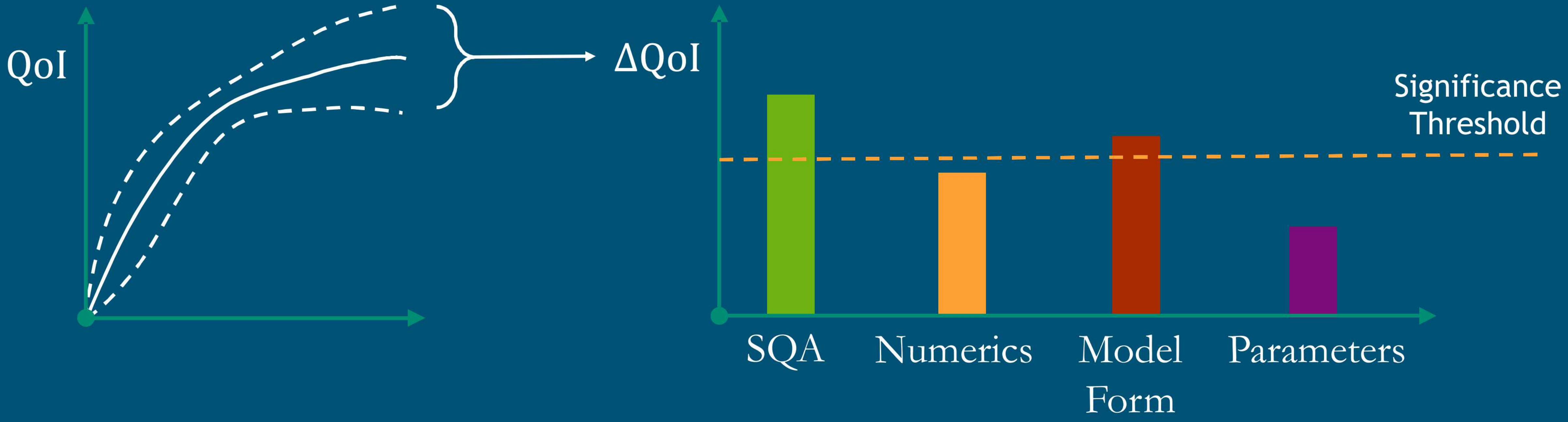

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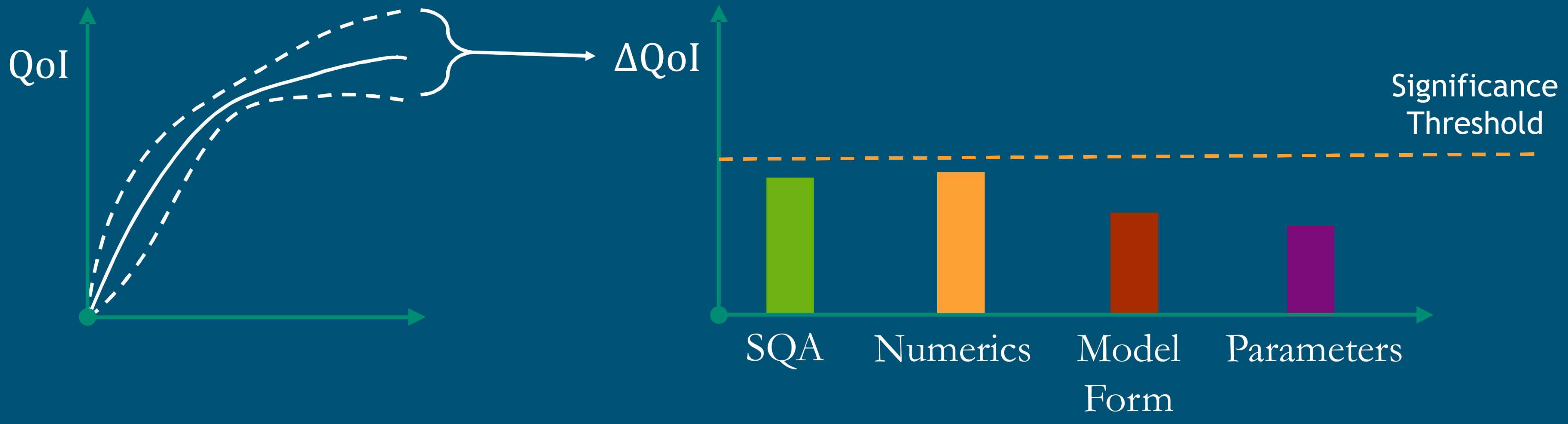


Summary and Future (1/2)

- MELCOR3 will lead the next generation of severe accident modelling
  - Algorithms are flexible and selectable/optimizable at run-time
  - Arbitrary field count and sources/field interactions
  - All terms errors
    - Are measured
    - Controlled/made small through dynamic meshing and time stepping
  - Measurement of all error terms separately allows per-term analysis of uncertainty/error contribution
  - Knowing which terms are contributing most to uncertainty/error allows focused effort of reduction to a set level of significance
  - **All pieces depend on one another**

Summary and Future (2/2)

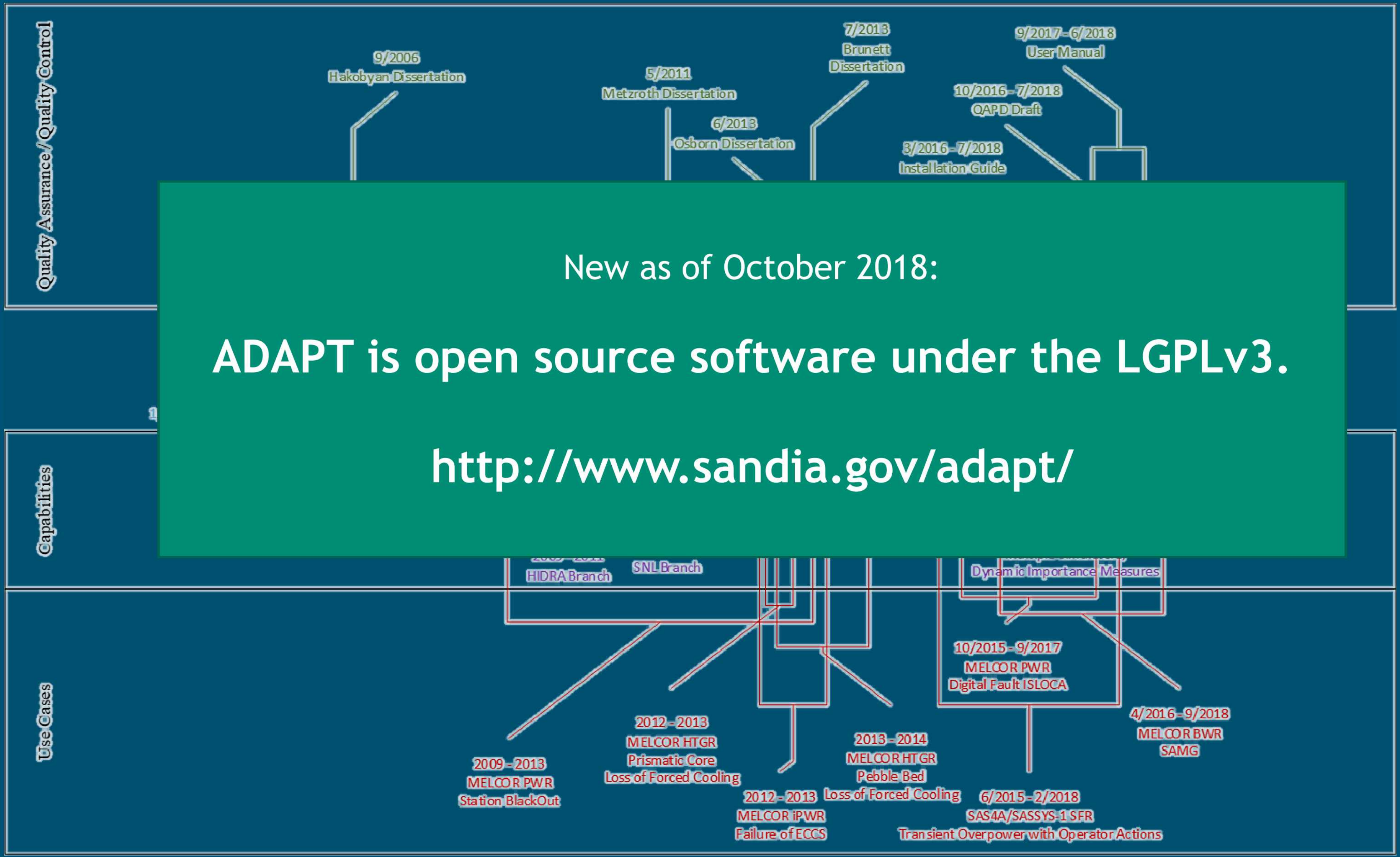
- Currently
  - Working on pilot code
  - Developing architecture in-code to effect the needed features
- Goal: completion of four test problems in Summer 2019

ADAPT

Purpose

- MELCOR3 is a physics simulator
  - Has length scales and time scales
  - Failure modes
  - Models parameters
- ADAPT is a dynamic event tree generator
  - Has events and probabilities with a map to simulator parameters
  - Needs a physics simulator to evolve toward a declared event
  - Adjusts simulator restart according to signaled event
    - Allows change in action
    - Change in parameters (epistemic or aleatory)
    - May map one-to-one or one-to-many
  - Launches child simulations with all adjusted restarts
  - Tracks parentage to build a tree of sequences informed by physics (unlike traditional PRA)
  - Aims for high-throughput computing (could be considered a cousin of HTCondor)

History



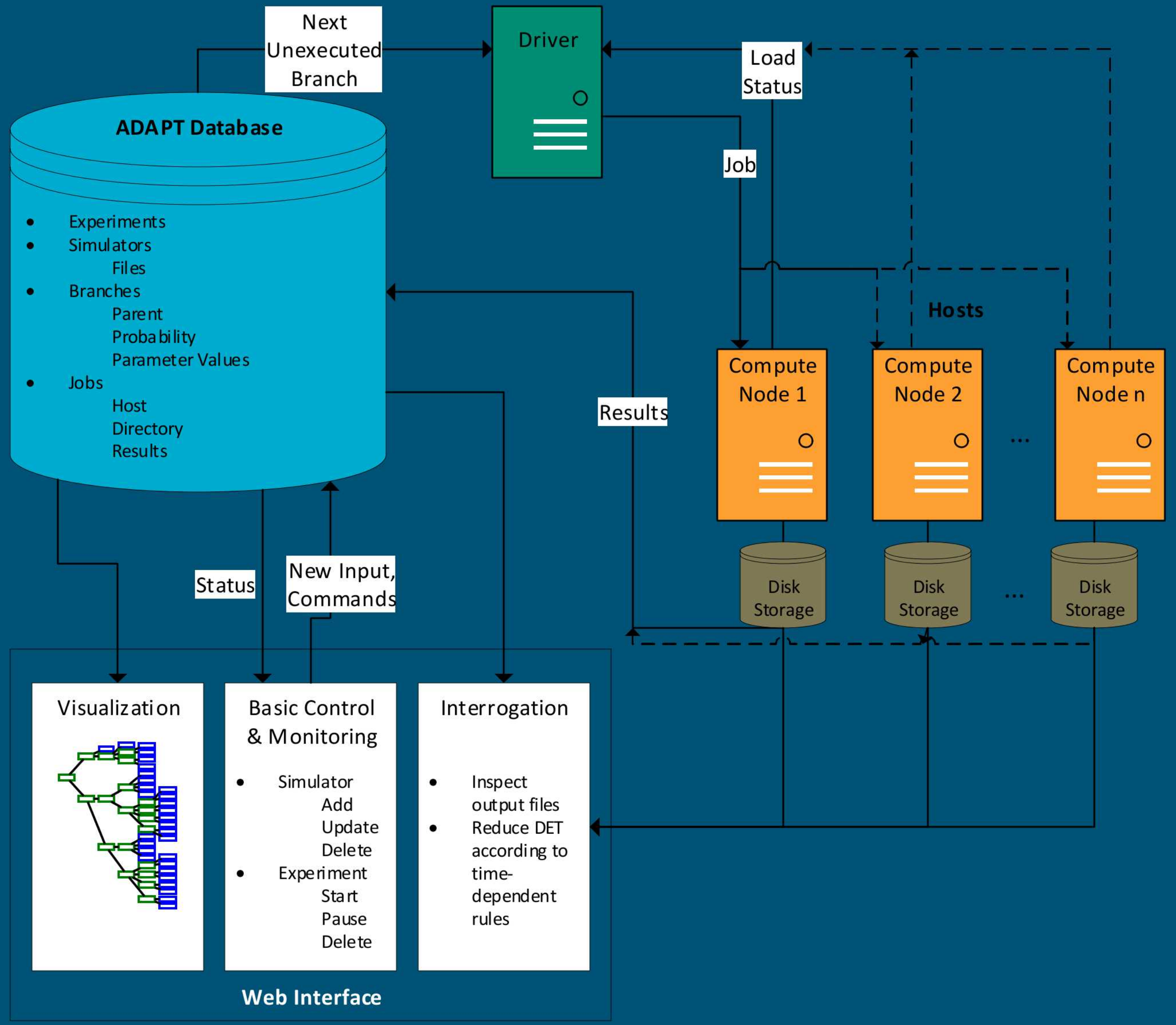
New as of October 2018:

ADAPT is open source software under the LGPLv3.

http://www.sandia.gov/adapt/

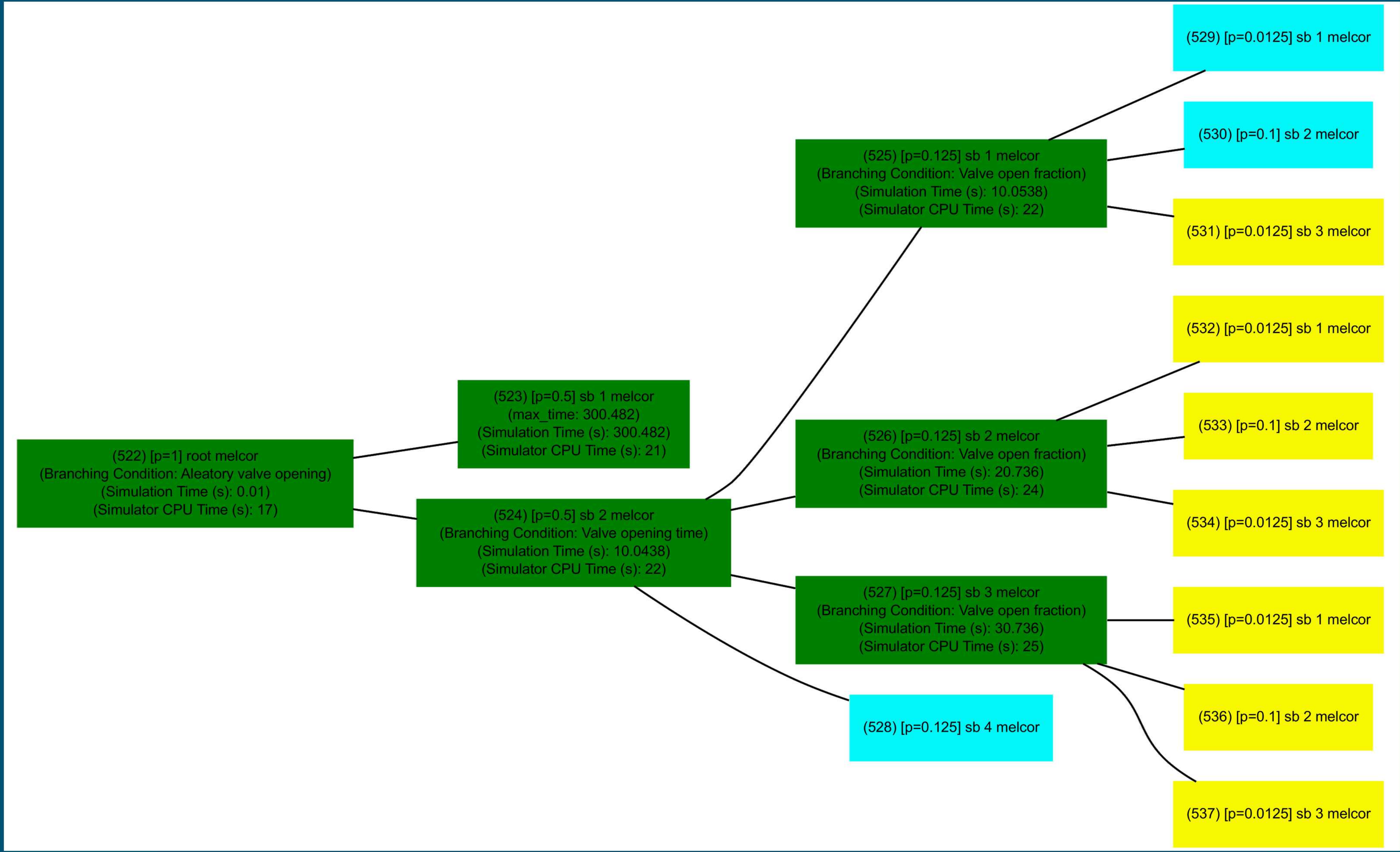
Design and Features (1/3)

- Implementation
  - Scheduler: Python
  - Database: MySQL (Python connector)
  - Web server: Python (cherrypy)
  - Web interface: pure HTML
- Future new version details
  - Release: TBD
  - Python 3 only
  - New web interface
    - Jinja2 templating engine
    - jQuery, LESS.js



Design and Features (2/3)

- Required Files
  - Wrapper
    - Controls ADAPT interaction with simulator(s)
    - Preparing input file, running simulator, post-processing, recording results
  - Branching Rules File (BRF)
    - Defines branching criteria, input to change, and probabilities
  - Restart File
    - Defines starting point of analysis (e.g., MELCOR restart file)
  - Template Simulator Input File (TSIF)
    - Contains all simulator parameters that may be modified by ADAPT
    - Parameter values replaced with ADAPT variables corresponding to BRF
    - Applying BRF to TSIF renders valid simulator input for an individual branch
  - Simulator executable
    - Must be capable of running on all assigned computation hosts


(522) [p=1] root melcor
(Branching Condition: Aleatory valve opening)
(Simulation Time (s): 0.01)
(Simulator CPU Time (s): 17)
(523) [p=0.5] sb 1 melcor
(max_time: 300.482)
(Simulation Time (s): 300.482)
(Simulator CPU Time (s): 21)
(524) [p=0.5] sb 2 melcor
(Branching Condition: Valve opening time)
(Simulation Time (s): 10.0438)
(Simulator CPU Time (s): 22)
(525) [p=0.125] sb 1 melcor
(Branching Condition: Valve open fraction)
(Simulation Time (s): 10.0538)
(Simulator CPU Time (s): 22)
(526) [p=0.125] sb 2 melcor
(Branching Condition: Valve open fraction)
(Simulation Time (s): 20.736)
(Simulator CPU Time (s): 24)
(527) [p=0.125] sb 3 melcor
(Branching Condition: Valve open fraction)
(Simulation Time (s): 30.736)
(Simulator CPU Time (s): 25)
(528) [p=0.125] sb 4 melcor
(529) [p=0.0125] sb 1 melcor
(530) [p=0.1] sb 2 melcor
(531) [p=0.0125] sb 3 melcor
(532) [p=0.0125] sb 1 melcor
(533) [p=0.1] sb 2 melcor
(534) [p=0.0125] sb 3 melcor
(535) [p=0.0125] sb 1 melcor
(536) [p=0.1] sb 2 melcor
(537) [p=0.0125] sb 3 melcor

Applications (1/3)

Years	Reactor Type	Accident Type	Simulator	References
2006-2011	PWR	SBO	MELCOR2	[1, 2, 3, 4, 5, 6]
2009	SFR	Aircraft Crash	RELAP5	[7]
2013	PWR	SBO	MELCOR2	[8, 9]
2013-2014	PWR	SBO	MELCOR2	[10, 11]
2014	PBMR	LOFC	MELCOR2	[12]
2015-2017	PWR	SBO	MAAP4	[13]
2015-2017	SFR	UTOP	SAS4A	[14, 15, 16]
2015-2018	PWR	ISLOCA	MELCOR2	[17, 18]
2016-2017	N/A	SNF Transport	Multiple	[19]

Applications (2/3)

- Example
  - MELCOR-RADTRAD ISLOCA test case compared at 66,076 branches finished
    - local (small) cluster on 132 (later 55) processors
    - HPCs on up to 3,000 processors
  - An HPC-run DET Snapshot
    - 697,663 branches finished
    - 1,448,618 identified
    - Over 46 Terabytes of data

Applications (3/3)

- DET breadth/depth can explode combinatorically!
  - HPCs needed for large number of branches
  - Load balancing is extremely important
- Active areas of effort
  - Visualization of large trees
  - Effective interrogation of data
  - Tools enabling extraction of insights from large sequence sets
  - Trimming branches based on metrics of importance and similarity (classification)

Summary and Future

- ADAPT is a DET Driver
  - Simulator agnostic
  - Job scheduler
  - Events based on evolution of physics
  - Naïve data visualization
- Future/Current work
  - Categorization of event types (e.g., epistemic, aleatory, decision)
  - Robust data visualization
    - Large sequence sets
    - Include event type information
  - Leverage Machine learning to elicit insights
  - New web interface
  - Code modernization

MELCOR3 and ADAPT

- MELCOR3
  - Next generation physics simulator
- ADAPT
  - Next generation dynamic event tree generator

Study Every Pebble, Walk Every Path, Limit No Horizon

MELCOR3 and ADAPT

Thank you.

Questions

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