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Two Problems for Benchmarking Numerical Codes for use in Potential HLW Salt Repositories

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Mechanical Behavior of Salt VIII

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NNSA National Nuclear Security Administration

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Outline

- Background & Motivation
- Descriptions of WIPP Experiments
- Benchmark Problem Definitions
- Advances in Hardware & Software
- Select Results for WIPP Isothermal Room D
  - Using benchmark definition
  - Using deviations from definition
- Summary & Conclusions

Background & Motivation

- Assurance of a HLW repository's performance & safety depends on numerical predictions of long-term repository behavior
- All aspects of the computational models used to predict the long-term behavior must be examined for adequacy
- This includes the computational software used to solve complex problems with many interacting nonlinearities that represent the geomechanics (for salt and other constituents) in the computational models
  - The numerical solution technique that solves the discretized equations over space and time, and
  - The numerical implementation of constitutive models that are used to represent the geo-material's behavior

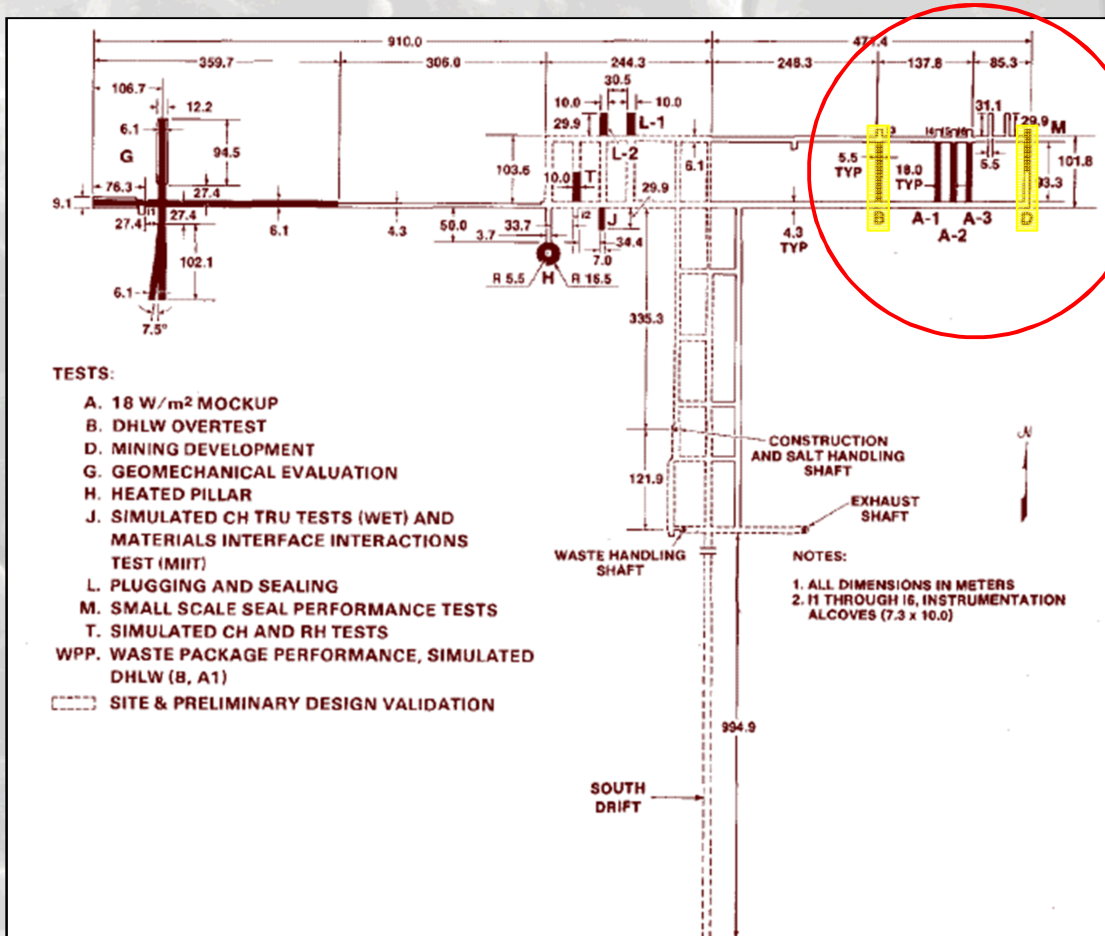
Background & Motivation (Cont'd)

- One way to evaluate the overall computational software is by the use of benchmark calculations whereby identically-defined parallel calculations are performed by two or more groups using independent but comparable capabilities (e.g., US-German JPIII)
- Benchmarking activities have been undertaken by SNL in the past (80's timeframe) under the auspices of the Waste Isolation Pilot Plant (WIPP)
- These were very valuable exercises that provided an excellent assessment of the computational capability of the time
- They also provided invaluable information on how benchmark problems should be formulated and carried-out to maximize their benefit
- But, these were prior to experiments being completed at WIPP

WIPP Experiments of Early 80's

Several Full-Scale Thermal-Structural Interactions (TSI) Experimental Rooms Started Being Fielded at the Waste Isolation Pilot Plant (WIPP) in the early 80's

Experimental WIPP Rooms D & B are of special interest & well-suited for benchmarking



Benchmarking using WIPP Rooms

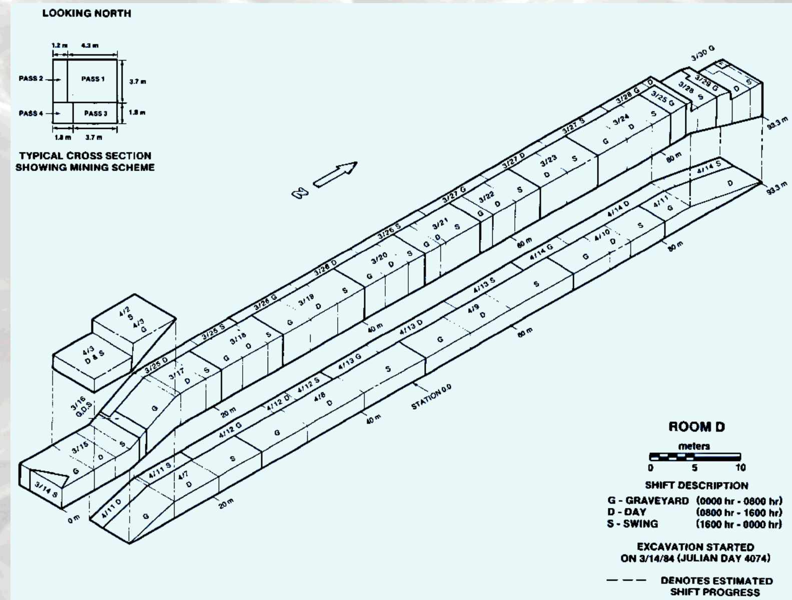
- Earlier WIPP benchmarking efforts, prior to the experimental rooms, relied solely on well-defined boundary-value problems
- Current benchmark problems are based on in-situ two full-scale tests conducted in the early 1980's at the Waste Isolation Pilot Plant (WIPP), located in Southeastern New Mexico, USA
  - The isothermal Mining Development Test – WIPP Room D
  - The heated Overtest for Simulated Defense High-Level Waste – WIPP Room B

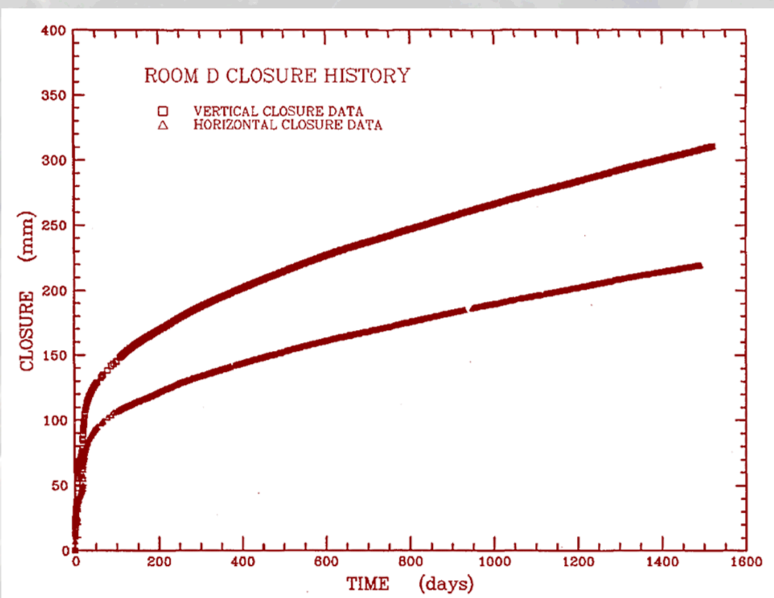
Room D

Room B

Complete Record of Room Closure Measurements

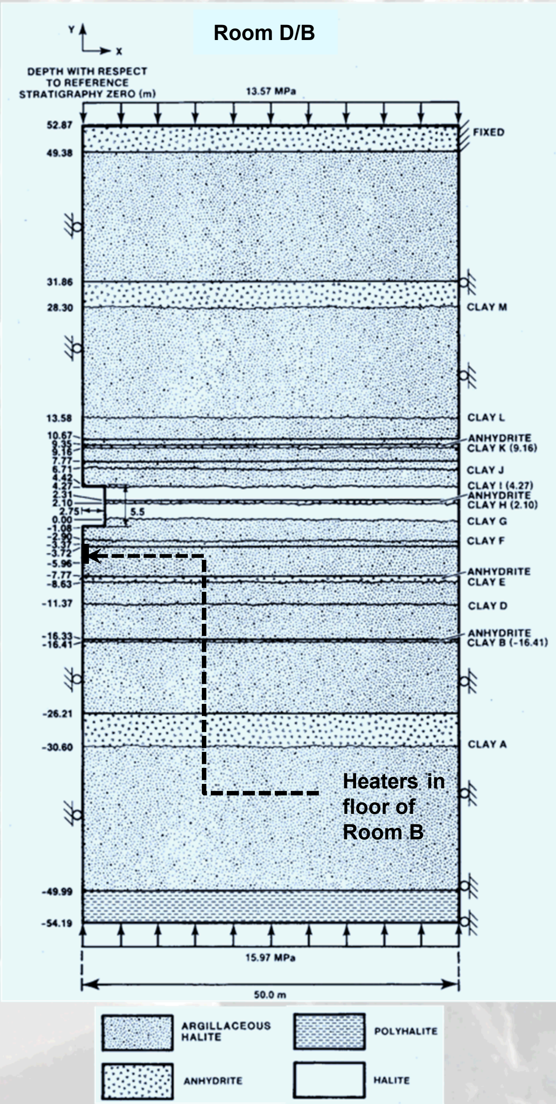
- Room excavation documented in detail – with complete face advance data
- Mining sequence closure gages were installed and manually read throughout the multi-pass excavation
- Manual mining sequence measurements started immediately after the mining face first pass had opened the station, i.e., within 1.0 m





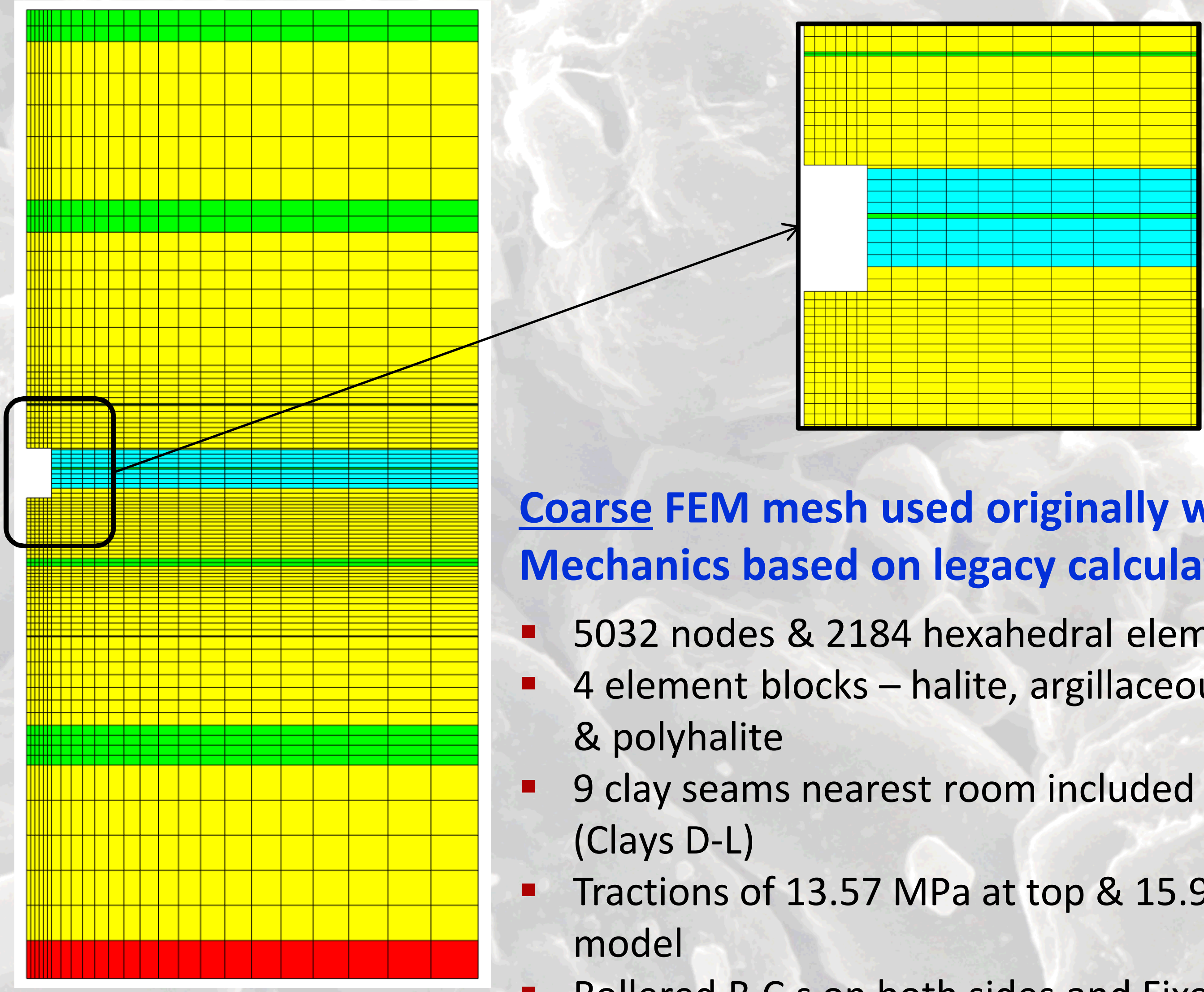
- Gage Linking – data from very early closures obtained manually during mining sequence could be linked to the later closures obtained manually at the temporary closure stations, and these could be linked in turn to even later closures obtained remotely from the permanent gage stations
- Resulted in transient response of room being well-captured and a high-quality complete data record

WIPP Rooms D & B Well-Suited for Benchmarking



- **Except for the heat load in Room B, both rooms are essentially identical**
  - Located in the same general area of WIPP
  - Relatively "isolated" from other workings
  - 5.5 X 5.5 m in cross-section (~100 m long)
  - At the same horizon and thus in the same vertical stratigraphic location
  - Tests conducted under rigorous Quality Assurance
  - Gages calibrated to NIST standards
  - Were extensively instrumented and data were taken for approximately 3.5 years (1300-1400 days) after excavation
  - Comprehensive datasets archived and available for benchmarking efforts
  - Figure shows idealized configuration used in legacy calculations of late-80's to early-90's

WIPP Room D Coarse Mesh – Similar to that Used in Legacy Calculations



Coarse FEM mesh used originally with Sierra Mechanics based on legacy calculations of rooms:

- 5032 nodes & 2184 hexahedral elements
- 4 element blocks – halite, argillaceous halite, anhydrite, & polyhalite
- 9 clay seams nearest room included as sliding surfaces (Clays D-L)
- Tractions of 13.57 MPa at top & 15.97 MPa at bottom of model
- Rollered B.C.s on both sides and Fixed B.C. near top right

Mechanical M-D Creep Modeling Parameters Used in WIPP Calculations

Note: Models based on details provided in Munson, 1997, *Int. J. Rock Mech. Min. Sci.* 34:2 233-247 (& supplemental information not provided there)

- Clean salt and Argillaceous Salt modeled with MD creep model with parameters shown here

	Parameters		Units	Salt
Salt Elastic Properties	Shear modulus	G	MPa	12,400
	Young's modulus	E	MPa	31,000
	Poisson's ratio	ν	–	0.25
Salt Creep Properties	Structure Factors	A_1	s^{-1}	8.386×10^{22} (1.407×10^{23})
		B_1		6.086×10^{6} (8.998×10^{6})
		A_2		9.672×10^{12} (1.314×10^{13})
		B_2		3.034×10^{-2} (4.289×10^{-2})
	Activation energies	Q_1	cal/mole	25,000
		Q_2	cal/mole	10,000
	Universal gas constant	R	cal/mol-ºK	1.987
	Absolute temperature	T	ºK	300
	Stress exponents	n_1	–	5.5
		n_2		5.0
	Stress limit of the dis-location slip mechanism	σ_0	MPa	20.57
	Stress constant	q	–	5,335
	Transient strain limit constants	M	–	3.0
		K_0	–	6.275×10^{5} (1.783×10^{6})
		c	$ºK^{-1}$	9.198×10^{-3}
	Constants for work-hardening parameter	α	–	-17.37 (-14.96)
		β	–	-7.738
	Recovery parameter	δ	–	0.58

Mechanical M-D Creep Modeling Parameters (Cont'd)

- Anhydrite and Polyhalite modeled with an elastic/perfectly-plastic Drucker-Prager criterion: $F = \sqrt{J_2} + aI_1 - C$

  where

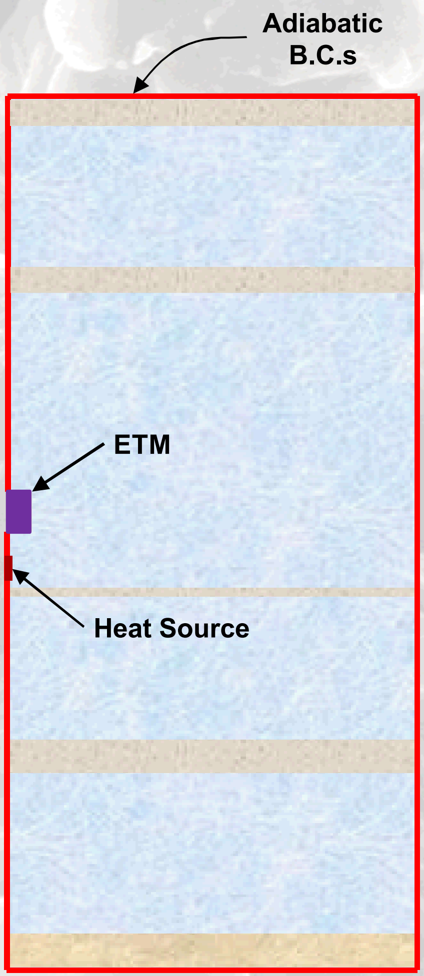
$$I_1 = \sigma_{kk}$$
$$J_2 = \frac{1}{2} s_{ij} s_{ji}$$
$$a, C = \text{material constants}$$

  with parameters as shown in table below.

Material	E (MPa)	ν	a	C (MPa)
Anhydrite	75,100	0.35	0.450	1.35
Polyhalite	55,300	0.36	0.473	1.42

- Clay seams modeled as sliding surfaces with M-C behavior: $\tau = \mu\sigma_n$ with μ=0.2
- Initial stress set to lithostatic stress varying linearly with depth

Thermal Modeling Parameters for Use in WIPP Room B Calculations



- All boundaries in "red" assumed to be adiabatic
- Boundaries sufficiently remote to preclude affecting room response for duration of simulation
- Entire formation prescribed to have an initial temperature of 300 K
- Heat is lost from below the floor by conduction through the salt to the room periphery where convective and radiative processes can become important
- The drift area (in "purple") assumed to consist of an "equivalent thermal material" (ETM)
- ETM has a constant high conductivity of 50 W/(m-K) & a high thermal diffusivity [C_P of 1,000 J/(kg-K) and a density of 1 kg/m^3]
- This presumably simulates convective & radiative heat transfer in the room by an equivalent conduction
- Heat loss from the room [Room B data report] was modeled with a time-dependent heat sink on the room periphery that varied with temperature rise
- Clay seams were neglected in thermal analyses

Thermal Modeling Parameters (Cont'd.)

Heat transfer through salt, anhydrite, and polyhalite modeled with a nonlinear thermal conductivity of the form:

$$\lambda = \lambda_{300}(300/T)^{\gamma}$$

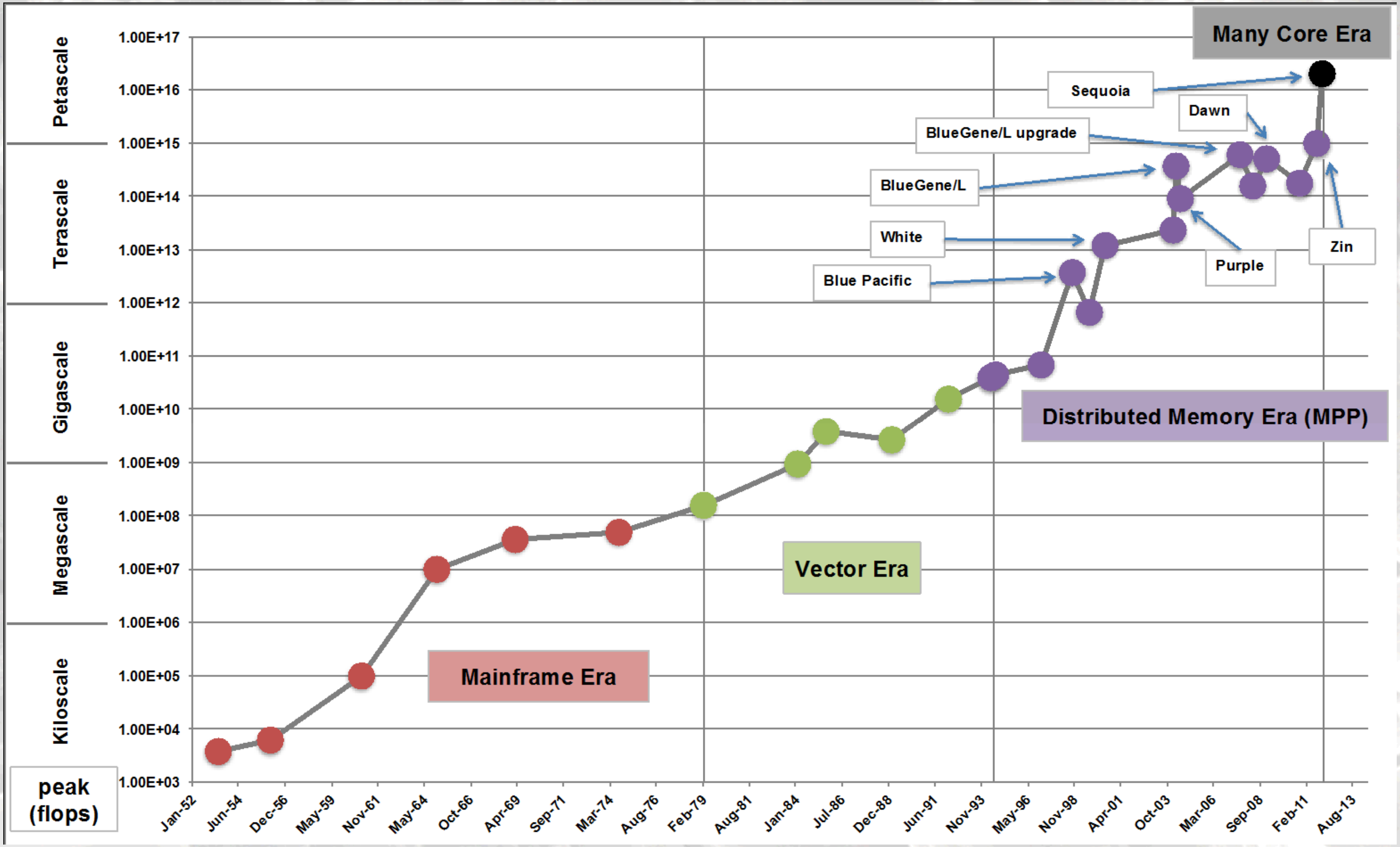
where λ is the thermal conductivity, T is the absolute temperature in Kelvin, and λ_{300} & γ are material constants.

The various parameters are given in table below and include:

C_P – the specific heat;
α – the coefficient of linear thermal expansion; and
ρ – the material density.

Material	C_P J/(kg-K)	α K^{-1}	λ_{300} W/(m-K)	γ	ρ kg/m^3
Salt	862	45×10^{-6}	5.4	1.14	2,300
Anhydrite	733	20×10^{-6}	4.7	1.15	2,300
Polyhalite	890	24×10^{-6}	1.4	0.35	2,300

Significant Advances in HPC Have Occurred From Mid-80's to Present

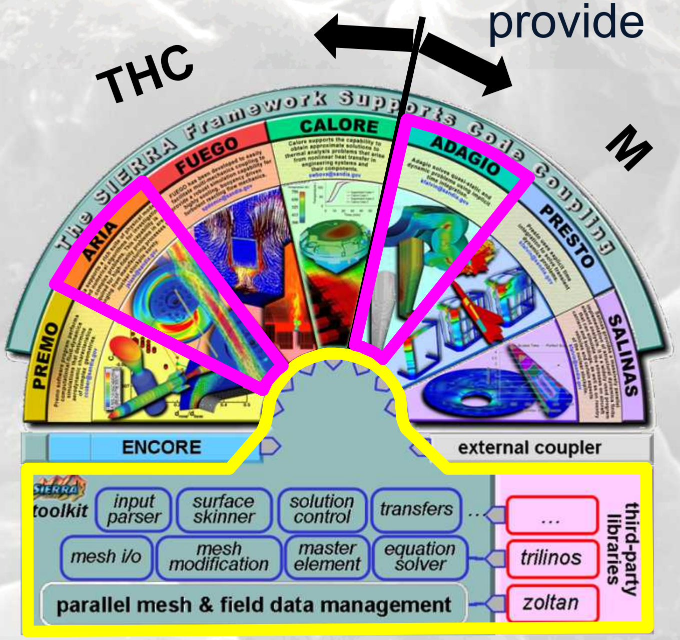


(Neely, R., "Supercomputing 101: A History of Platform Evolution and Future Trends," *CSGF HPC Workshop,* LLNL-PRES-657110, *July 17, 2014)*

Sierra Mechanics

Past/Present: State-of-the-Art integrates single physics codes to achieve coarse spatial and time scale simulation…

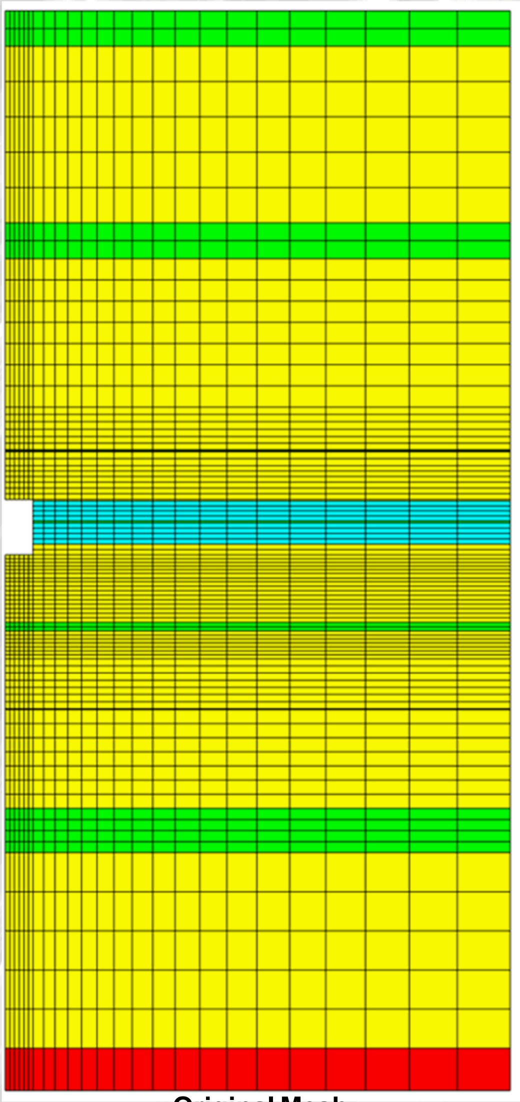
Future: New Software Platforms – e.g., SIERRA Mechanics leverages 15+ years of ASC development to provide



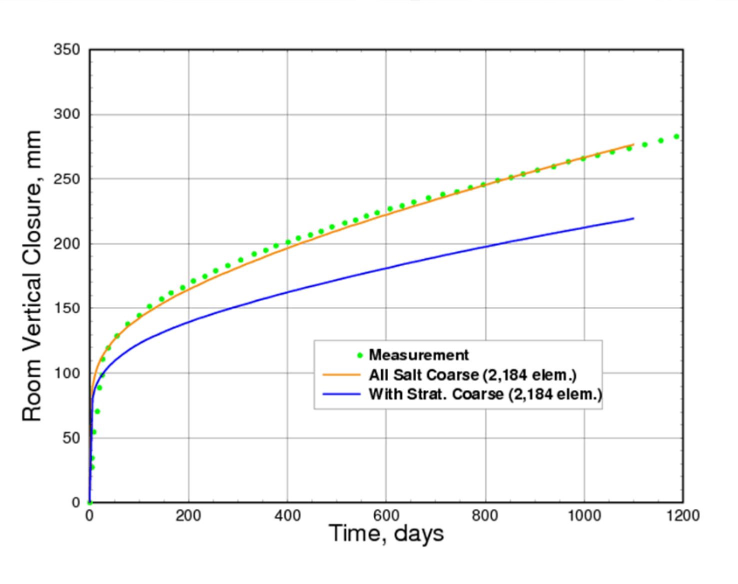
- Framework for coupled multi-physics simulations in a massively parallel environment
  - Scalability from 1 to thousands of processors on a variety of platforms
    - Launching point for fully integrated THMC coupling with adaptive solution control

(Edwards, H.C., & Stewart, J.R. 2001. SIERRA: A Software Environment for Developing Complex Multi-Physics Applications. In K.J. Bathe (ed.), *First MIT Conference on Computational Fluid and Solid Mechanics*. Amsterdam: Elsevier)

Room D Model Matching Capability Available in Mid-80s to early 90s

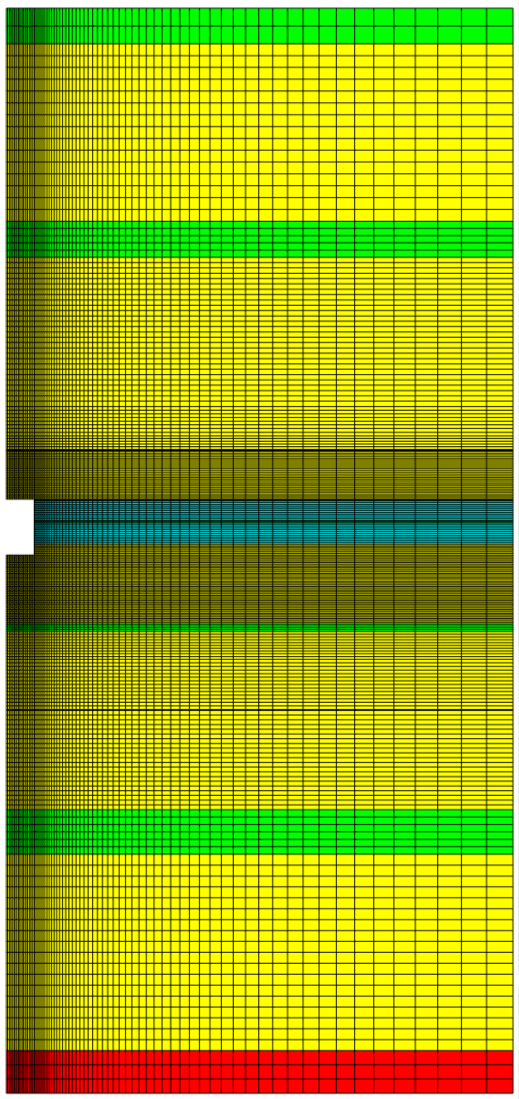


Original Mesh

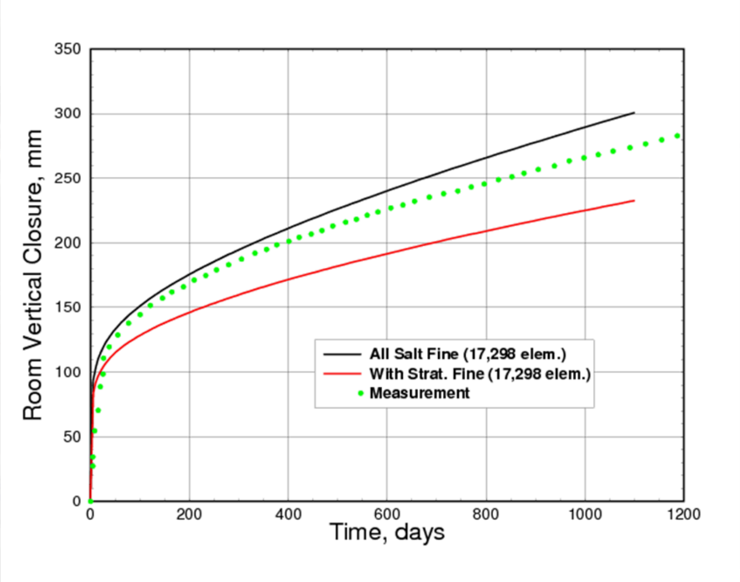


- Original mesh is coarse by today's standards, but similar to what was possible in the mid-1980s to early 1990s, in terms of computational capability
- With this mesh, the computed vertical closure is comparable to the measured vertical closure (using an all-salt stratigraphy, as was apparently done in past)
- With this mesh and the complete stratigraphy, the computed vertical closure is less than the measured closure

Refining the Room D Model in Line with Current Generation Capability



Refined Mesh



- New generation of computational tools allows more refined mesh, in line with current practice/ standards, to better-capture stress gradients
- Mesh shown here includes roughly an order-of-magnitude increase in the number of elements compared to the coarse mesh (something not possible with machines of mid-80s to early 90s)
- With the refined mesh, the computed vertical closure is greater than that computed with the coarse mesh, for either the all-salt or with complete stratigraphy cases
- Computed results bracket the measurements

Summary & Conclusions

- Original coarse mesh with various details available (transmitted to JPIII German partners as a starting point)
- Additional information needed for the benchmarking effort has been identified and made available
- Using the original mesh density with an all-salt idealization, the computed Room D vertical closure with SIERRA Mechanics agrees reasonably well with the measurements
- Refinement of Room D model to conform with modern standards/ practice leads to greater vertical closure than measurements for the all-salt idealization but less than measurements for the full stratigraphy
- Appears that in legacy model, MD parameters (& other features, e.g., μ for clay seams) were calibrated to match the tests using a relatively coarse mesh that was acceptable at the time
- This remains an open question that we hope to answer under current JPIII benchmarking efforts
- Implies that a common refinement of the room model among the various partners is probably needed to be able to make appropriate comparisons between the results of all the participant in the benchmark study