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Coupled Model for Thermal-Hydrological-Mechanical Processes in a High-Level Radioactive Waste Repository in Salt

J. Guadalupe Argüello, J. E. Bean, J. F. Holland, & J. S. Rath*

Sandia National Laboratories

*(with contributions from numerous others currently at or retired from Sandia, as well as various contributions over the years from RESPEC)

U.S. Nuclear Waste Technical Review Board Meeting

Albuquerque, NM

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Outline

- **Brief Overview of Sandia's Historical Efforts Related to Salt Repositories (Geomechanics Perspective)**
  - WIPP Full-Scale Thermal-Structural Interactions (TSI) In-Situ Tests
  - Technology developed for WIPP
  - Verification & Validation (V&V) of Legacy Technology
- **Next-Generation High-Performance Computing (HPC) Efforts/Technology**
  - Software & Hardware Advances
  - Multi-Physics Coupling
  - SIERRA Mechanics
  - Current and Future V&V efforts
- **Additional Work on Salt for High-Level Waste (HLW) Repository**
  - Constitutive Modeling
  - International Collaborations
- **Demonstration Problems**
  - US-German Isothermal Free Convergence (IFC) & Heated Free Convergence Probe (HFCP) Benchmark Problems
  - Demo Problem on a Generic HLW Repository
- **Summary**

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Brief Overview of Sandia's Historical Efforts Related to Salt Repositories (Geomechanics Perspective)

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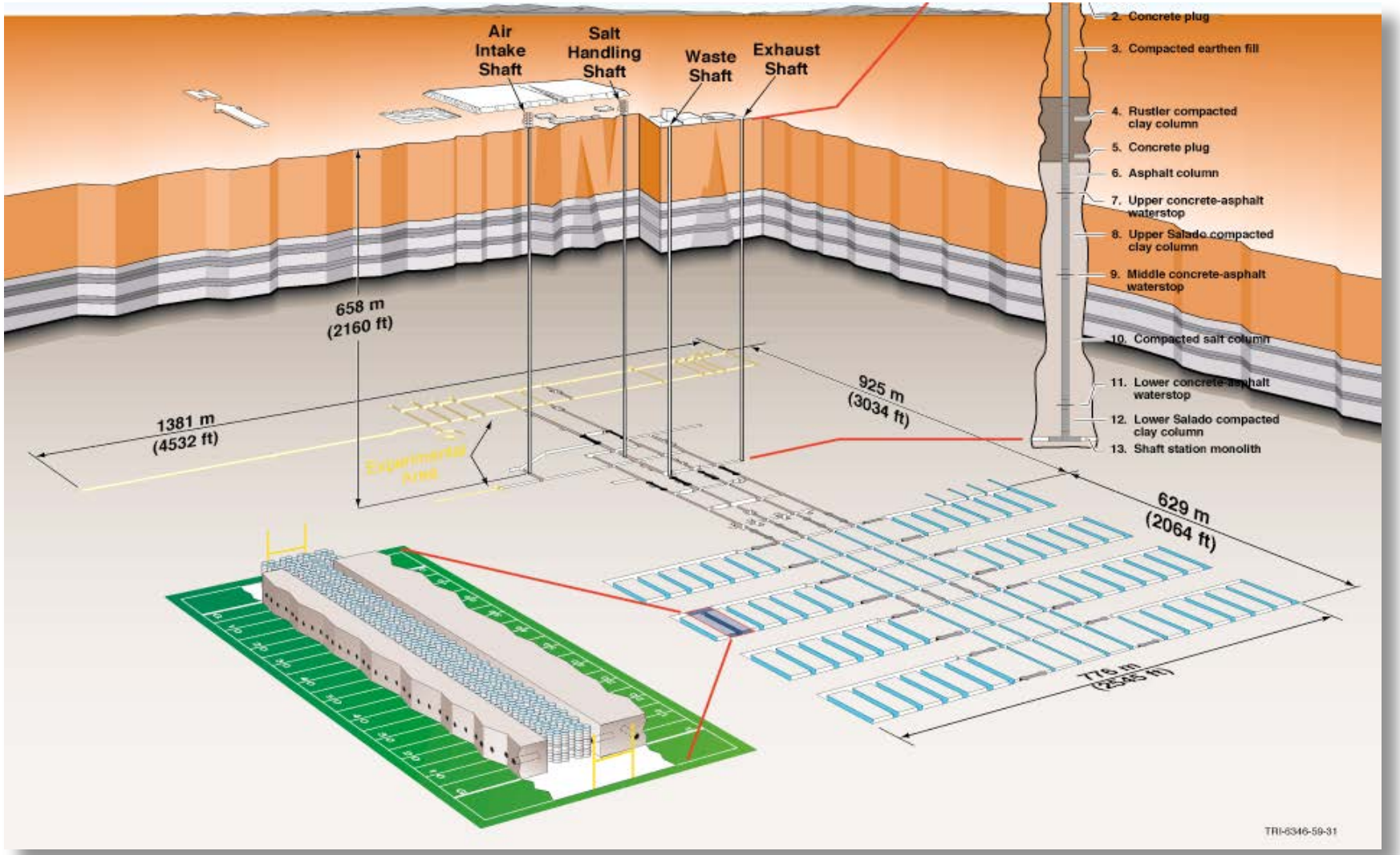
WIPP Schematic



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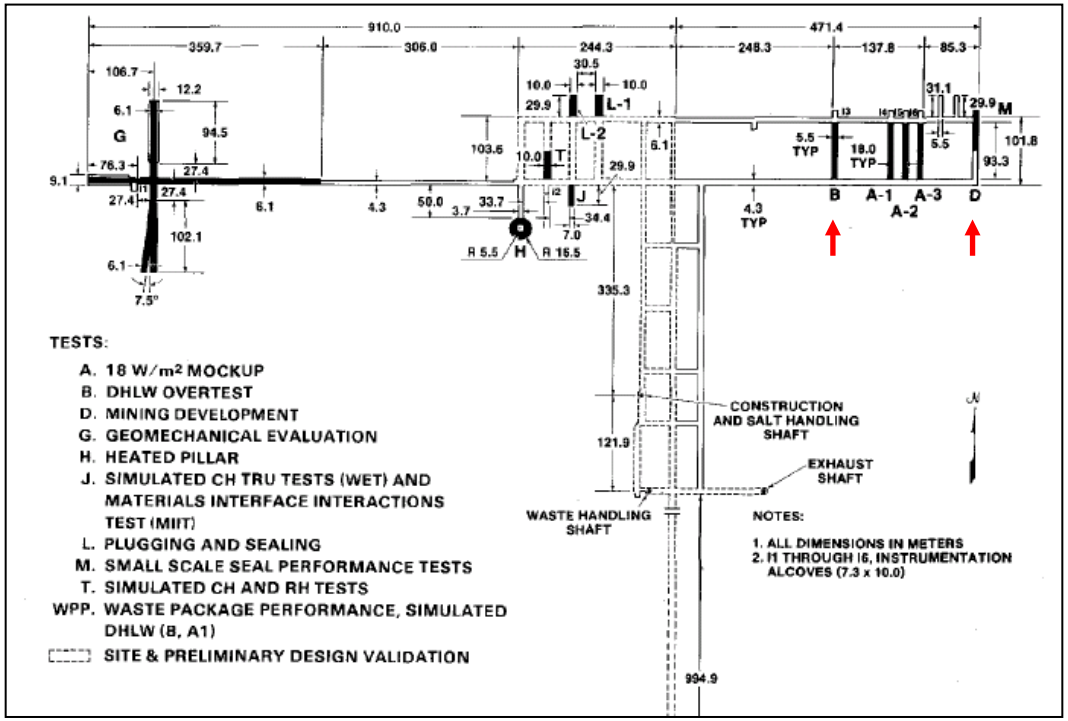
Past Salt Geomechanics Efforts Conducted at WIPP

- Early-on Sandia tasked with developing technology for predicting the geomechanical response of rock salt (thermo-mechanical – e.g. creep models, Sancho, Coyote, SPECTROM-32, SPECTROM-41, SANTOS, JAC3D, etc.)
- TSI Full-Scale Experimental Rooms Fielded at WIPP; with one of the objectives being the evaluation of the predictive models and techniques being developed



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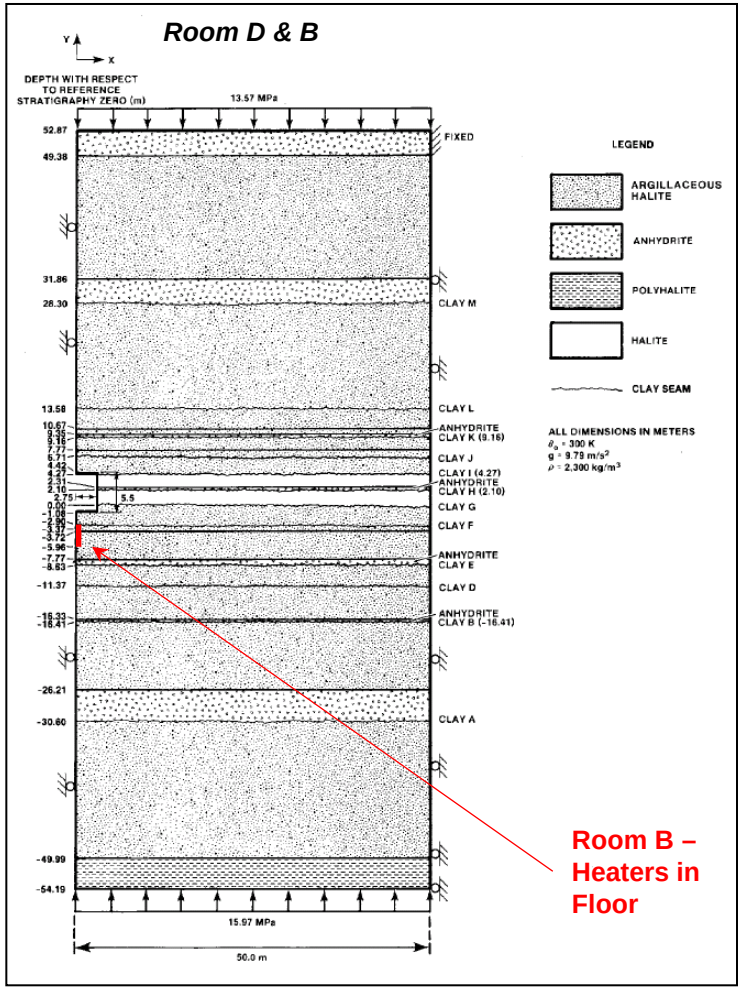
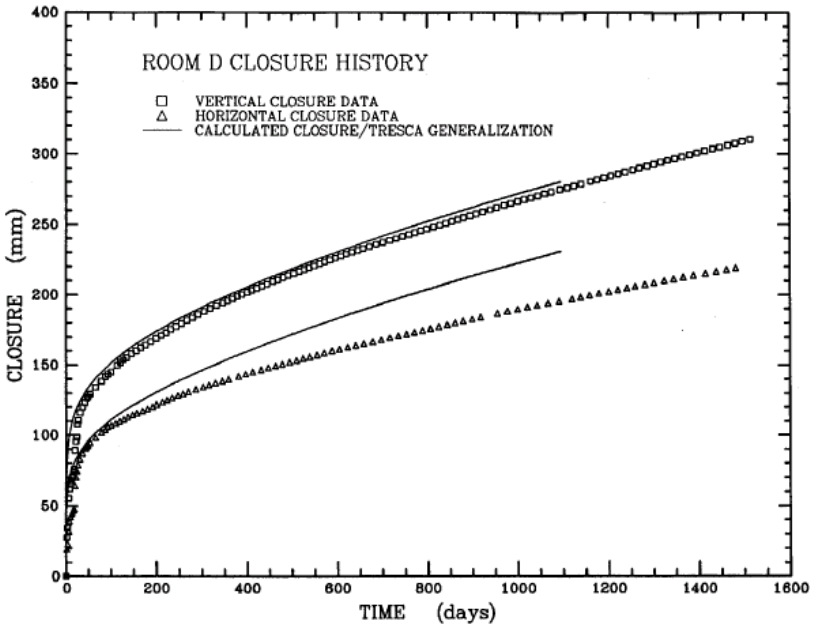
Room D Field Test at WIPP

- **Room D – Mining Development Test Data vs. Calculated Results (Isothermal Room)**



Mining development test (Room D) : in situ data report (March 1984-May 1988) : Waste Isolation Pilot Plant (WIPP) thermal/structural interactions program.

Munson, Darrell Eugene, Jones, Robert L., Hoag, David Leverett, Ball, John R. 1988. SAND88-1460, Sandia National Laboratories, Albuquerque, NM



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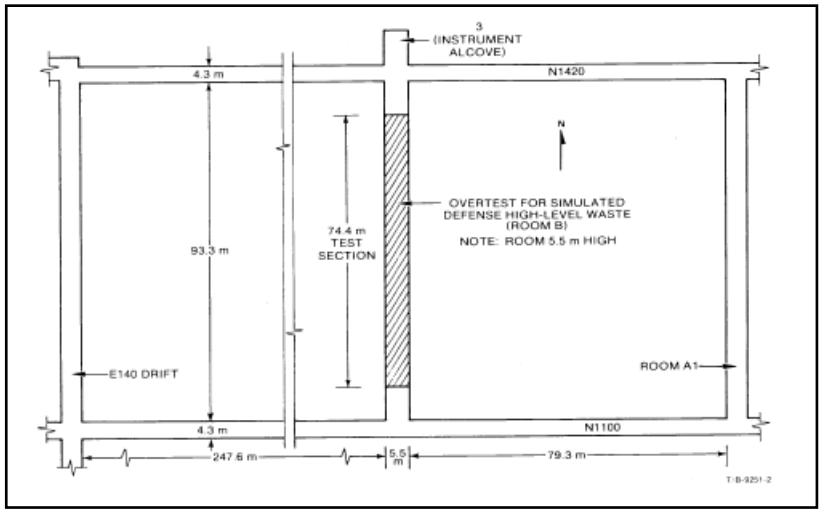
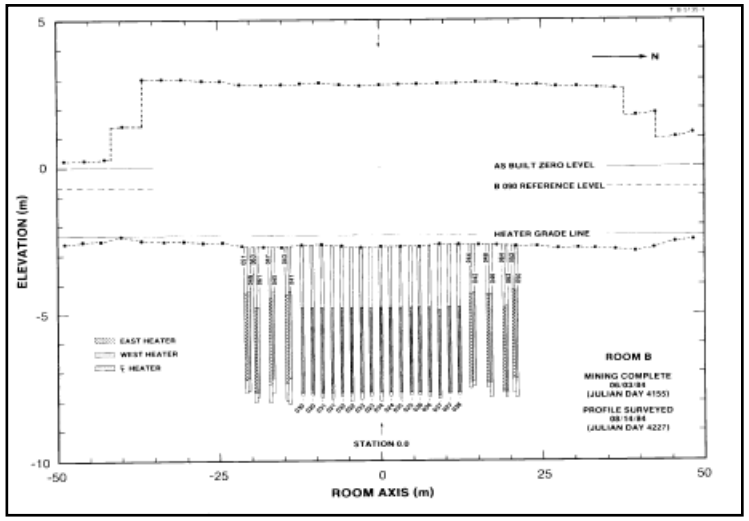
Room B Field Test at WIPP



Overtest for Simulated Defense High-Level Waste (Room B): In Situ Data Report (May 1984 – February 1988)

Waste Isolation Pilot Plant (WIPP) Thermal/Structural Interactions Program

Darrell E. Munson, Robert L. Jones, John R. Ball,
Robert M. Clancy, David L. Hoag, Sharon V. Petney



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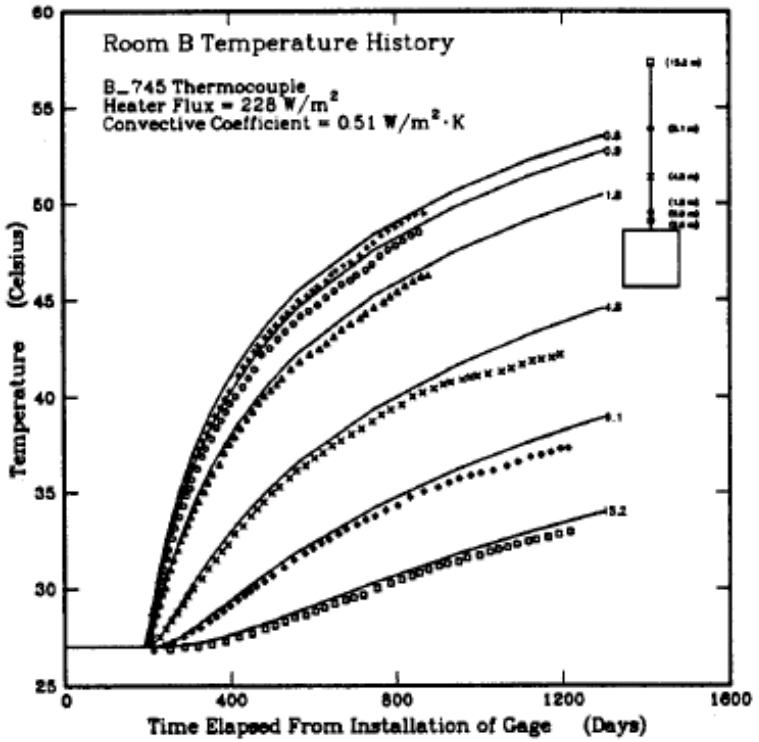
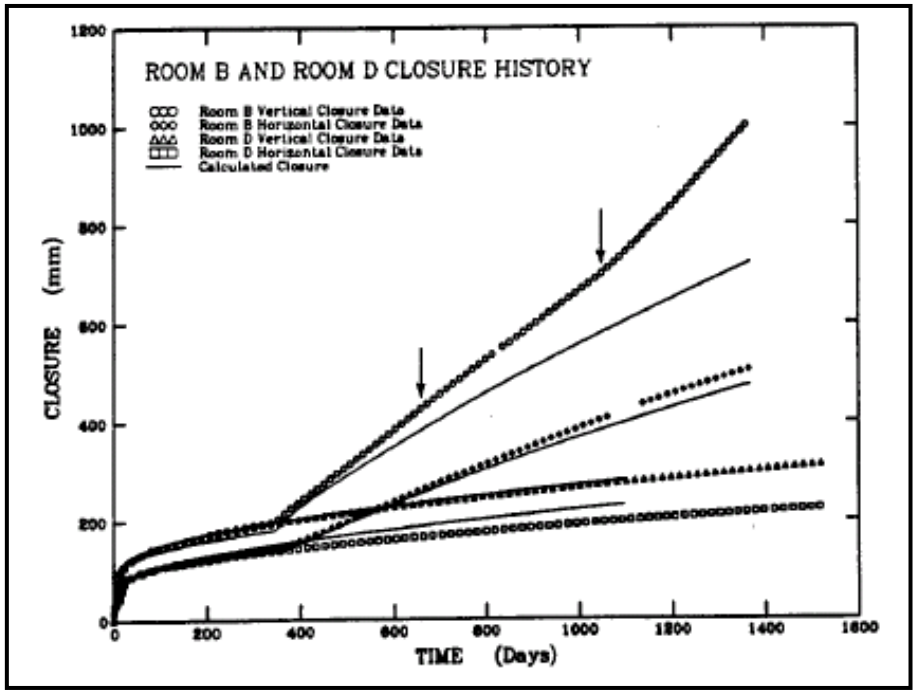
Room B Field Test at WIPP

Room B – Over-test for Simulated Defense High-Level Waste (Heated Room of Same Geometry and at Same Horizon as the Isothermal Room D)





Various other WIPP experimental configurations were also simulated for comparison with measurements*

* [Munson, D. E., "Constitutive Model of Creep in Rock Salt Applied to Underground Room Closure," *Int. J. Rock Mech. Min. Sci.,* Vol. 34, No. 2, pp. 233-247, 1997]

Next-Generation HPC Efforts/Technology

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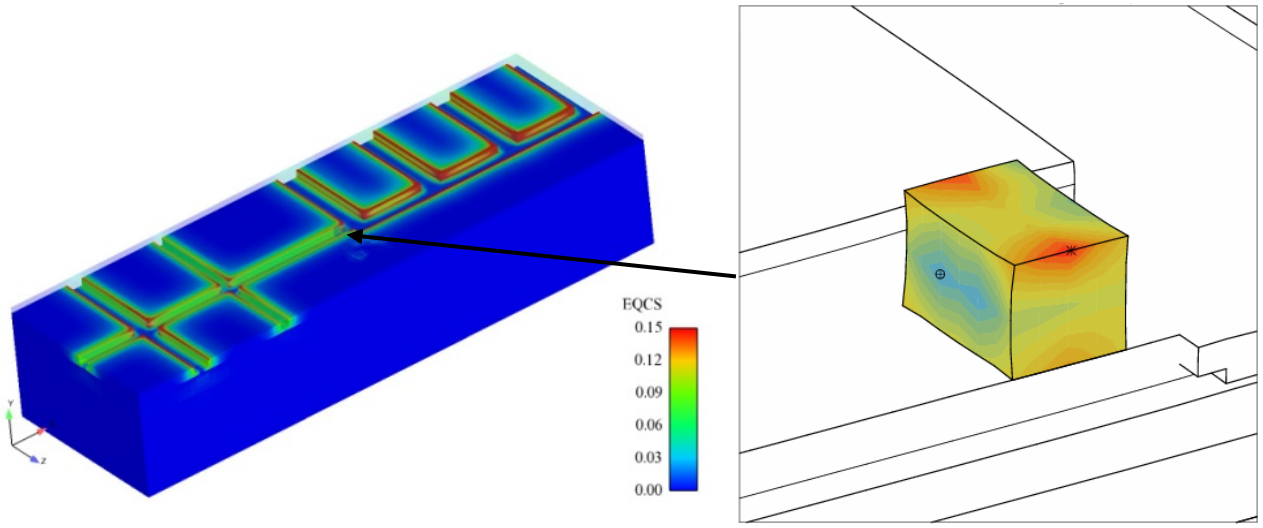
Next Generation of Coupled Simulations

- **Since mid-1980's, ~30 years of software and hardware advances have transpired**
- **Sandia has built a new generation of massively-parallel multi-physics capabilities into a single computational framework to support the Sandia engineering sciences mission (ASC)**
- **These tools recently being adapted for simulating coupled geomechanics for a waste repository setting**
  - LDRD (laboratory-directly research & development)
  - UFD (used fuels disposition campaign)



Panel Entryway Seal

- ***Is Room Closure Inhibited by Seal?***
- ***What Sorts of Loads Induced on Seal?***

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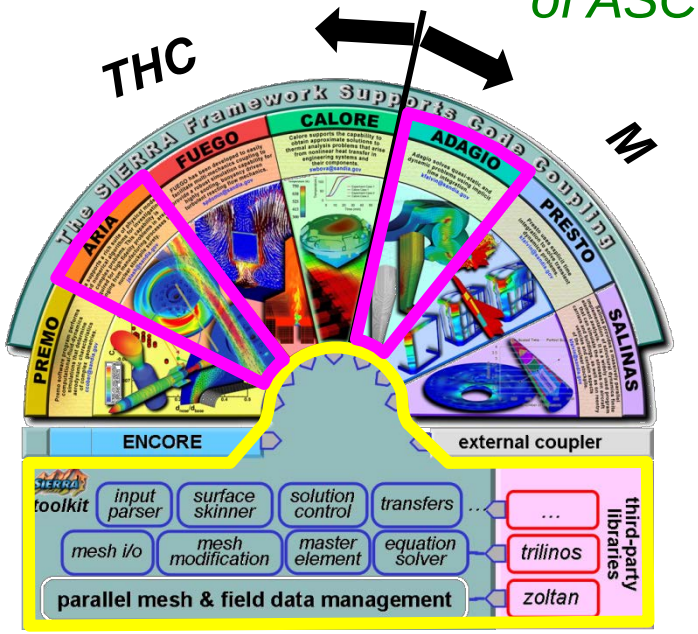
SIERRA Mechanics

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

Future: *SIERRA Mechanics leverages >10 years of ASC development providing:*



- *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.]

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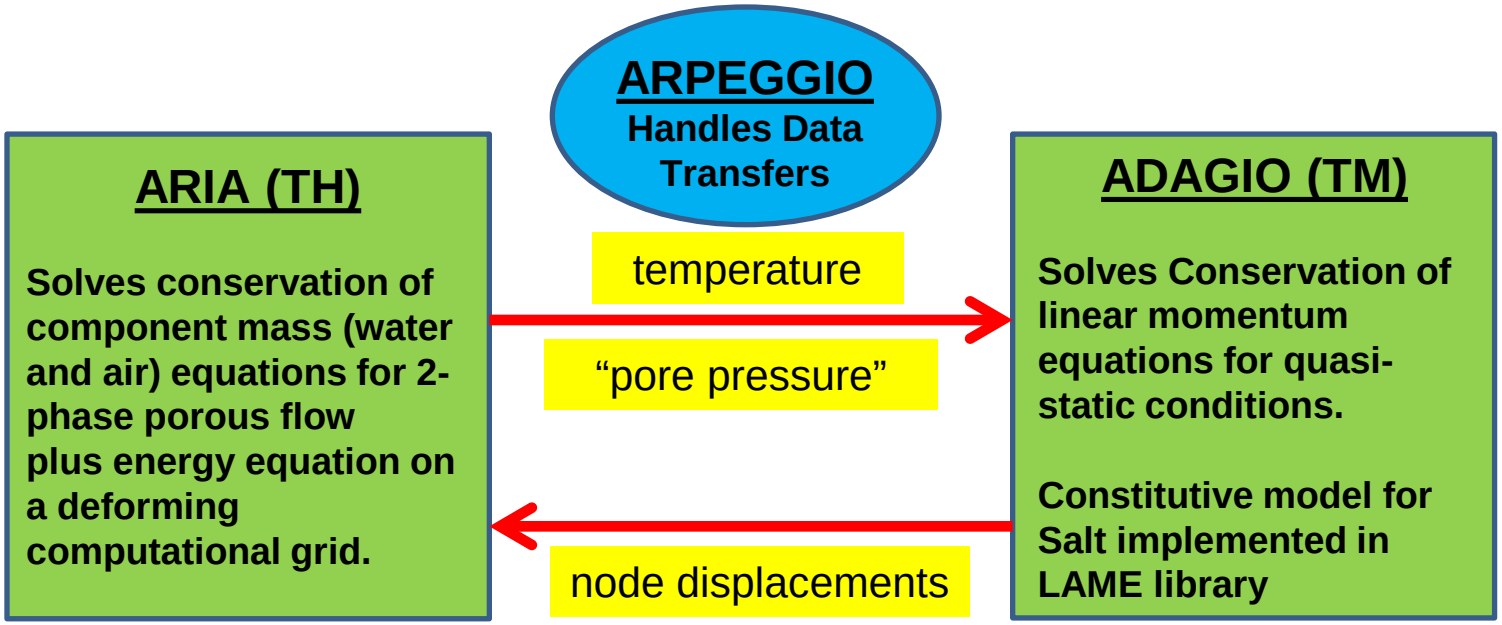
SIERRA Mechanics Coupling Between Application Codes



- **Temperatures are used in the constitutive equations for the salt materials. If needed (hydrological processes), pore pressures are used to compute effective stresses from the total stresses in ADAGIO.**
- **Constitutive model for salt is implemented in LAME library – within ADAGIO**
- **Node displacements from ADAGIO are used to update the ARIA geometry. (Porosity, thermal conductivity, and intrinsic permeability of crushed salt backfill, if hydrologically present, are adjusted accordingly.)**

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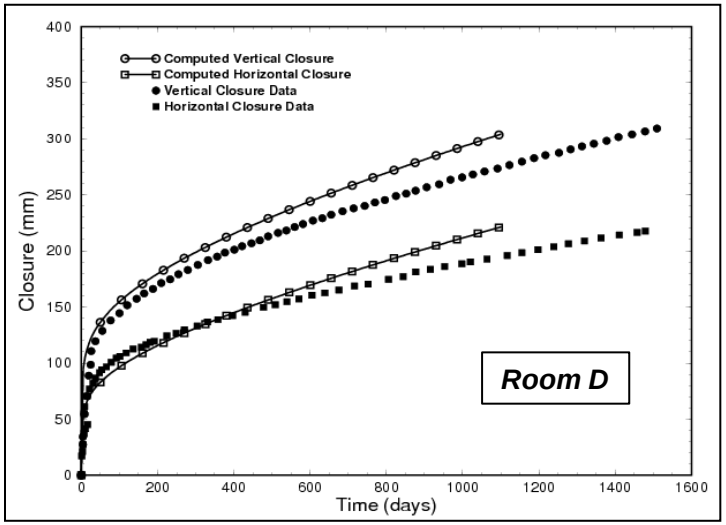
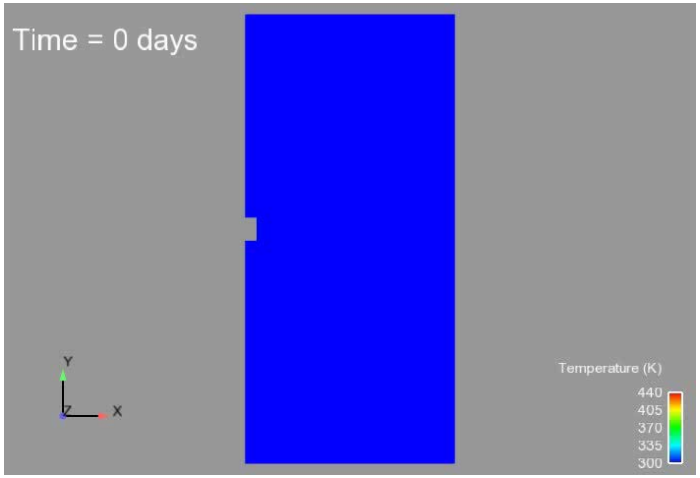
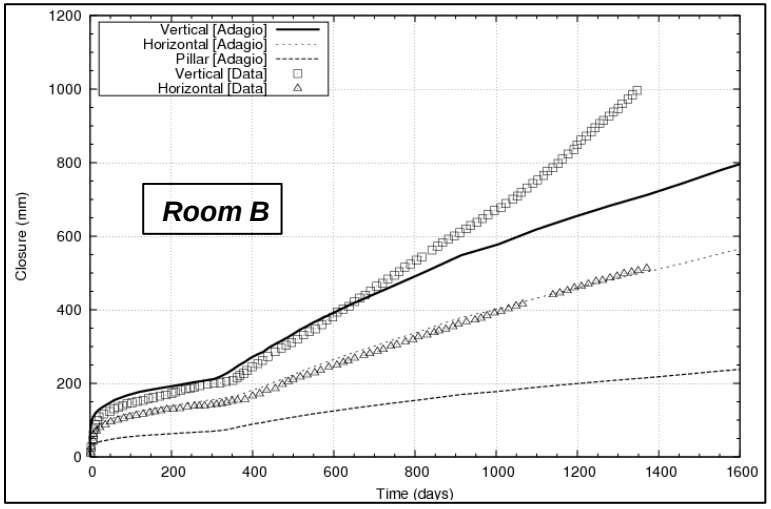
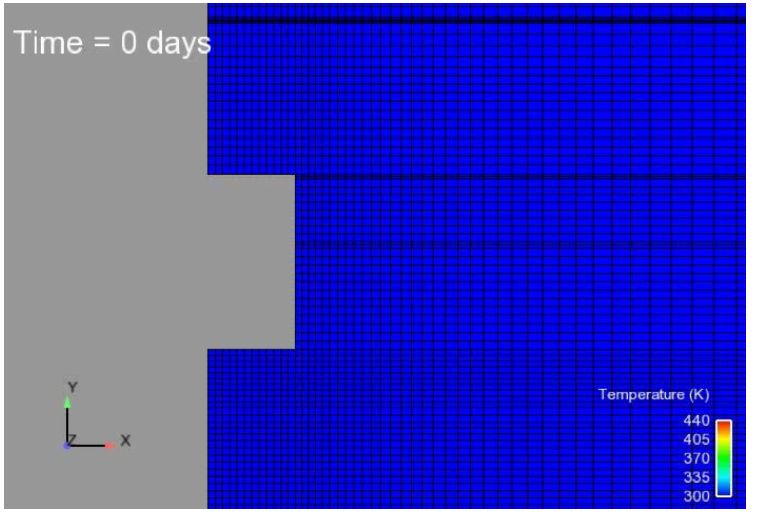
Preliminary Validation of SIERRA Mechanics Against WIPP Rooms D & B Data









[Argüello, J.G., and J.S. Rath, 2012. SIERRA Mechanics for Coupled Multi-Physics Modeling of Salt Repositories. In P. Bérest, M. Ghoreychi, F. Hadj-Hassen, & M. Tijani (Eds.), *Mechanical Behavior of Salt VII.* Boca Raton: Balkema.]

Additional Work on Salt for HLW Repository

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Modeling Salt Behavior Correctly

- Salt constitutive modeling is very important (forms basis for US-German collaborations)
- Our constitutive model development efforts stopped in mid-90's; German development continued
- The Multi-mechanism Deformation (MD) model is currently in use in our HPC codes (some initial work on "MDCF," but not mature)
- Need to assess the international capabilities
- Examine potential development of our model & evaluate other existing models
- Identify best features and deficiencies

Room Temperature Triaxial Test Sample of WIPP Salt at 3.0 MPa Confining Stress

Multi-mechanism deformation (MD) model:

$$\dot{\varepsilon}_s = \sum_{i=1}^{3} \dot{\varepsilon}_{s_i}$$

$$\dot{\varepsilon}_{ij}^{c} = F\,\dot{\varepsilon}_s \frac{\partial \bar{\sigma}}{\partial \sigma_{ij}}$$

$$F = \begin{cases} e^{\Delta[1-\zeta/\varepsilon_t^*]^2}, & \zeta < \varepsilon_t^* \\ 1 & \zeta = \varepsilon_t^* \\ e^{-\delta[1-\zeta/\varepsilon_t^*]^2} & \zeta > \varepsilon_t^* \end{cases}$$

$$\dot{\zeta} = (F-1)\dot{\varepsilon}_s$$

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Participants in Current U.S.-German Joint Project III

- **"Comparison of current constitutive models and simulation procedures on the basis of model calculations of the thermo-mechanical behavior and healing of rock salt"**
- **Previous phases (i.e., JPI & JPII) looked at behavior without heat**
- **The German project partners are each represented by:**
  - Dr. Andreas Hampel, Scientific Consultant
  - Dr. Wolfgang Minkley, Institut für Gebirgsmechanik GmbH
  - Ms. Alexandra Pudewills, Institut für Nukleare Entsorgung (INE), Karlsruher Institut für Technologie
  - Prof. Dr. Reinhard Rokahr, Institut für Unterirdisches Bauen, Leibniz Universität Hannover
  - Prof. Dr. Karl-Heinz Lux, Lehrstuhl für Deponietechnik und Geomechanik, Technische Universität Clausthal
  - Prof. Dr. Joachim Stahlmann, Institut für Grundbau und Bodenmechanik, Technische Universität Braunschweig
- **Sandia National Laboratories joined as a partner in FY2010**

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Overview of Joint Project III – Current Project

Current Joint Project on the "Comparison of current constitutive models and simulation procedures on the basis of model calculations of the thermo-mechanical behavior and healing of rock salt"

Joint Project III (Oct. 01, 2010 – Sept. 30, 2013 (general) / Jan. 31,2014 (Hampel)):

- *Check & compare the suitability of the models for the simulation of the thermo-mechanical behavior and damage reduction (sealing/healing) of rock salt (Comparisons of the simulation results with each other and with in-situ data.)*

Thermo-Mechanical behavior and sealing/healing of salt.

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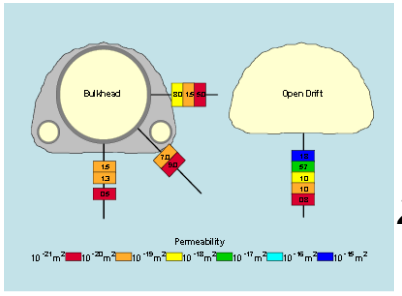
Joint Project III Target Simulations for Comparison with Data

- ***In-situ calculation object "Bohrlochkonvergenz" (borehole convergence) in the Asse mine***
- ***In-situ calculation object "Erhitzerversuche" (heater experiments) in the Asse mine***
- ***In-situ calculation object "Dammjoch" (bulkhead) in the Asse mine***



1911: drift excavated

1914: a 25 m long section lined with a cast steel tube, residual gap filled with concrete

2008?: permeability measurements (gas injection)

- ***Recent additions to three originally proposed Joint Project III benchmark problems and extension (BMWi) of project for Germans***
  - ***In-situ isothermal WIPP Room D and heated WIPP Room B simulations***
  - ***Additional laboratory testing of both clean and argillaceous WIPP salt samples – needed for German constitutive models***

Demonstration Problems

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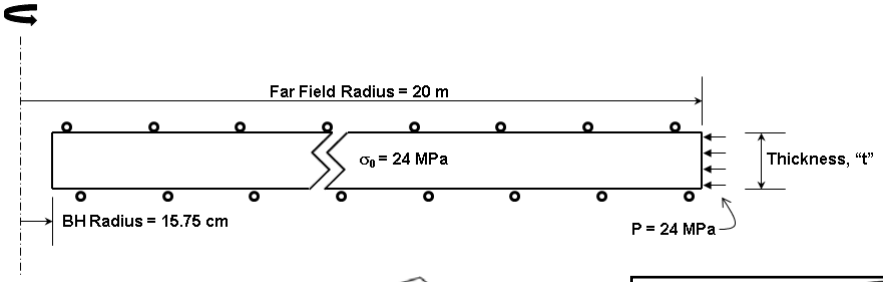
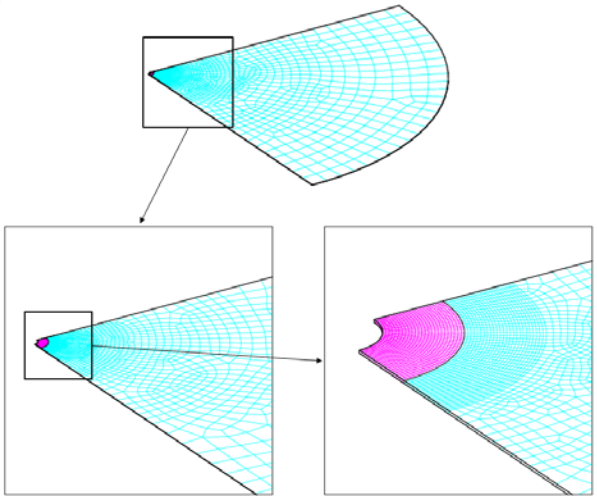
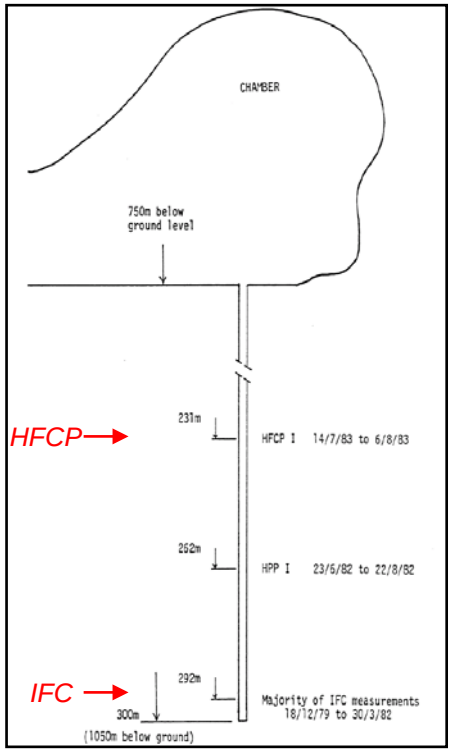
First JPIII Target Simulation (IFC) for Comparison with Data

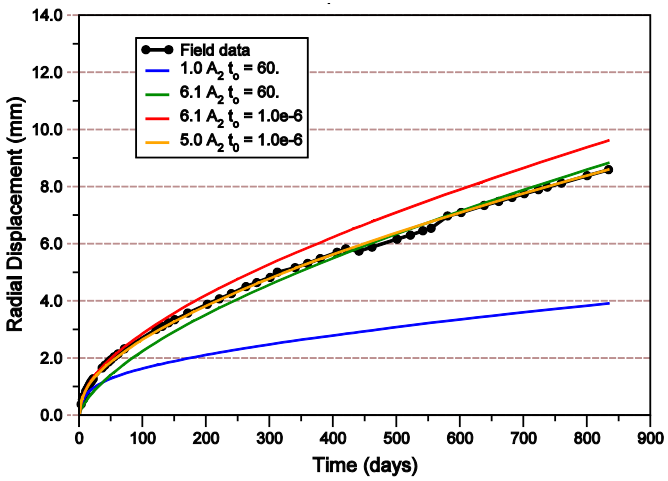




Isothermal Model Configuration, Mesh Details, and Boundary Conditions – "Asse Speisesalz" properties



Borehole Closure Results with Varying Secondary Creep Parameter. Fitting of this parameter is allowed to match data; subsequent thermo-mechanical (heater) analyses used this fitted value without further changes.



[Argüello, J.G., Holland, J.F., and Bean, J.E., 2012. International Benchmark Calculations of Field Experiments at the Asse Salt Mine. FCRD-UFD-2012-000374, Sandia National Laboratories (SAND2013-8193), Albuquerque, NM.]

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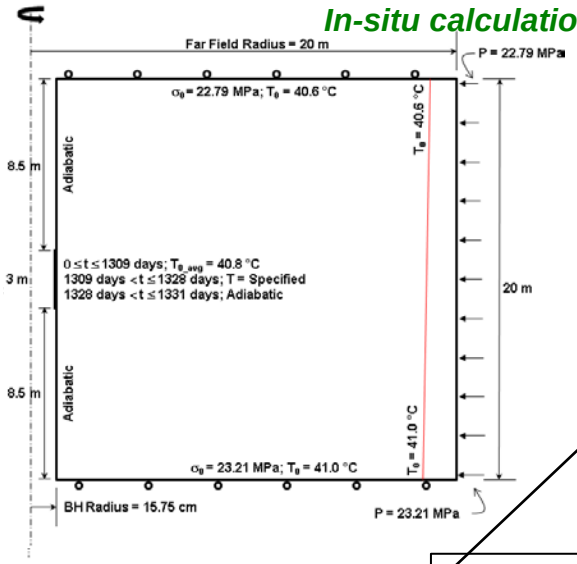
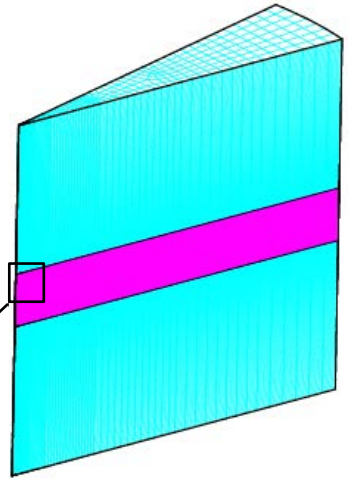
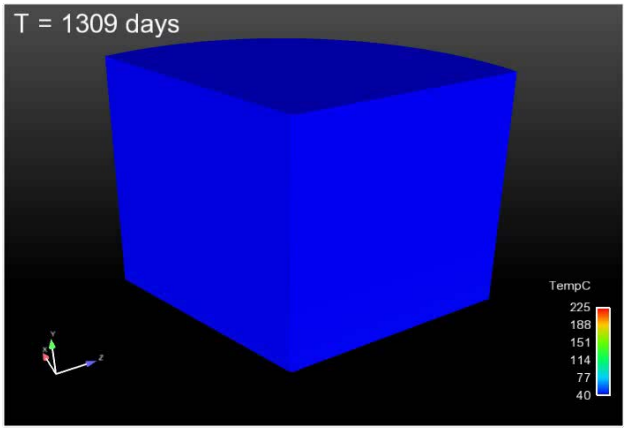
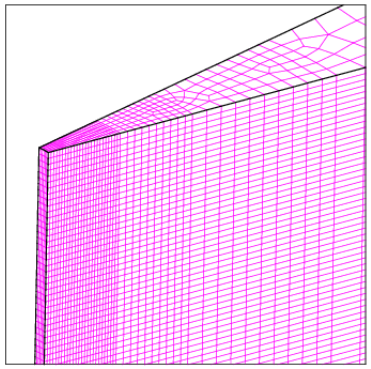
Second JPIII Target Simulation (HFCP) for Comparison with Data

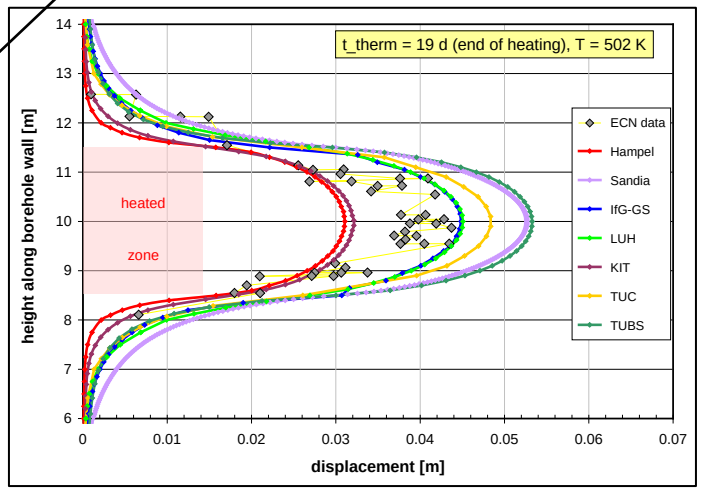
In-situ calculation object "Erhitzerversuche" (heater experiments) in the Asse mine

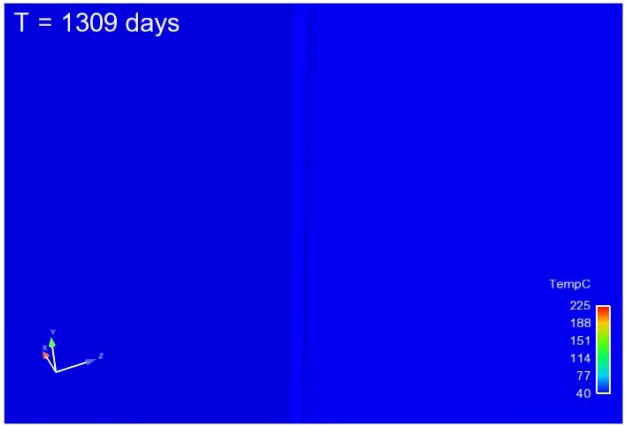












[Hampel, A., et al., 2013. Benchmark Calculations of the Thermo-Mechanical Behavior of Rock Salt – Results from a US-German Joint Project. (ARMA-13-456). *Proc. American Rock Mechanics Association (ARMA) 47th US Rock Mechanics / Geomechanics Symposium, 23-26 June 2013.* San Francisco: American Rock Mechanics Association.]

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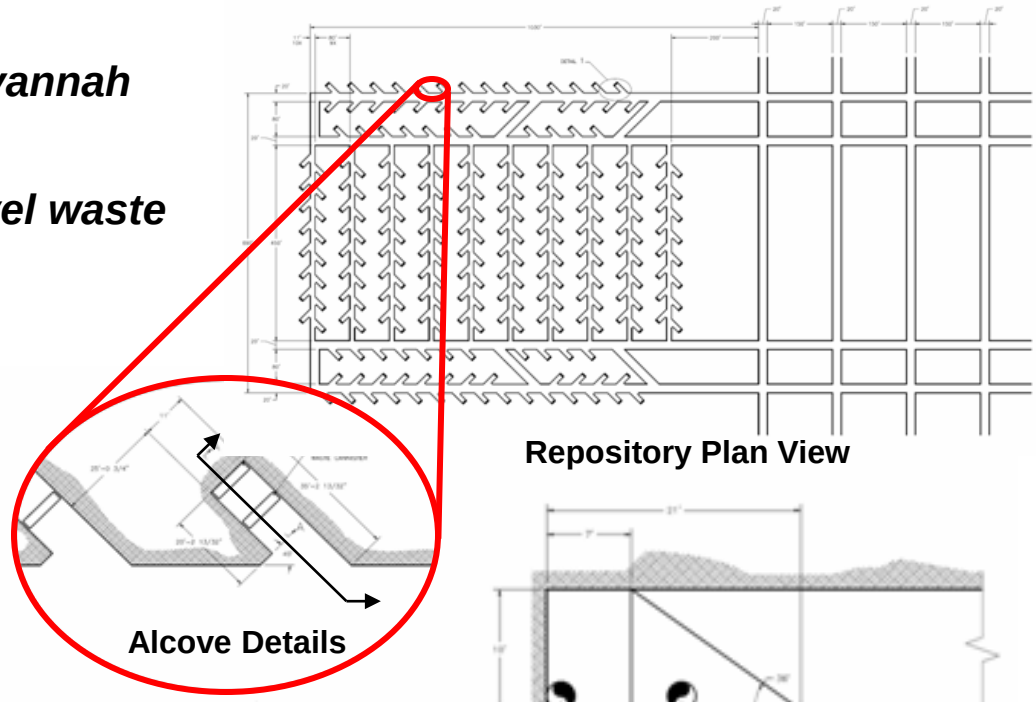
Coupled Thermal-Mechanical Simulation of Generic HLW Salt Repository

Sample Geometry:

- ***Configuration based on a 2008 Savannah River study***
- ***Vitrified borosilicate glass high level waste canister with output 8.4 kW***

Technical challenges:

- ***High Thermal Gradients***
- ***Temperature dependent material properties***
- ***Large Deformation Salt Creep behavior***
- ***Contact modeling with heat conduction and load transfer***
- ***Long duration simulation to room closure***



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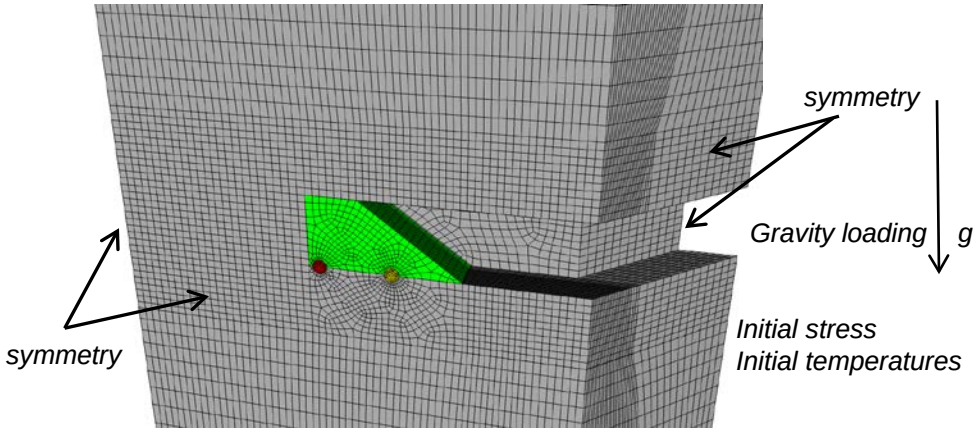
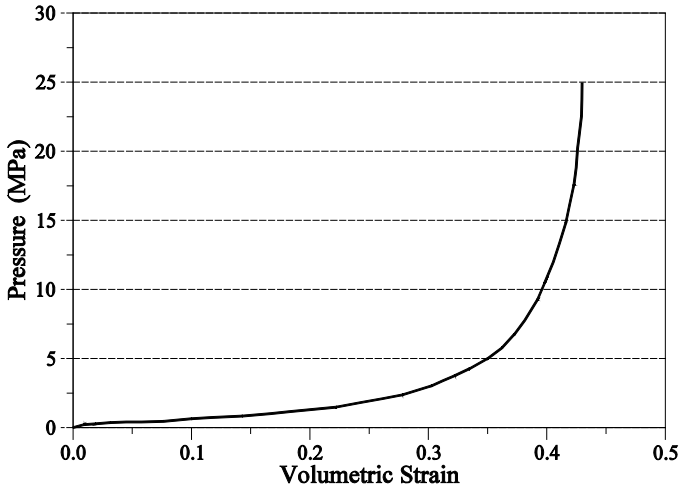
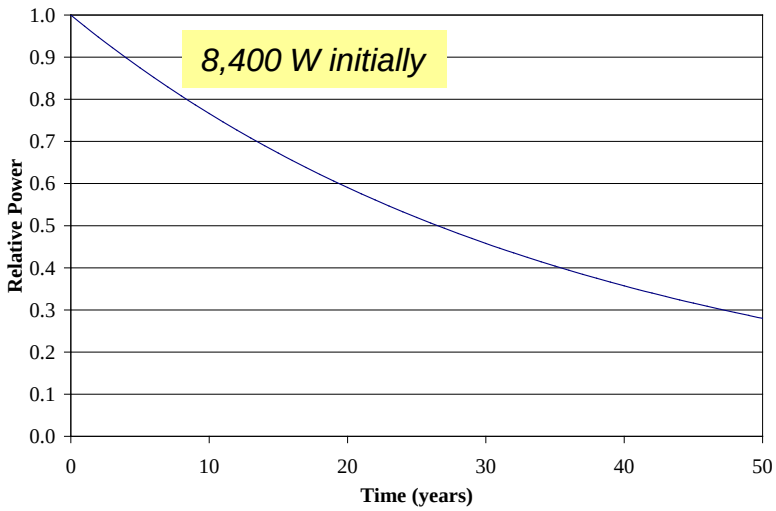
Generic HLW Salt Repository Problem Definition



Thermal and mechanical boundary conditions



Experimental pressure-volume strain curve for crushed salt at 200 C



Normalized power curve for HLW waste canister

Temperature dependent salt conductivity:

$$\lambda_{salt}(T) = \lambda_{300}\left(\frac{300}{T}\right)^{\gamma}$$

where:

- λ_{300} *= material constant, 5.4 [W/m/K]*
- γ *= material constant, 1.14*
- T *= temperature [K]*

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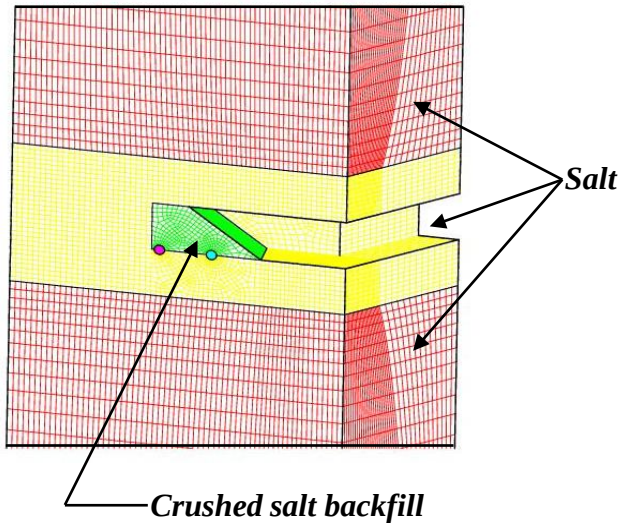
Sierra Mechanics Thermal-Mechanical Simulation of Generic HLW Salt Repository



- *Three-dimensional fully coupled thermal/mechanical analysis*
- *Massively Parallel Calculation - 96 processors*
- *Dissimilar meshes and domains for thermal and structural mechanics*
- *Contact surfaces used for both thermal and structural problems*

Thermal Analysis Features:

- *904736 nodes / 864927 elements*
- *Contact surfaces used to accommodate heat conduction between contacting surfaces (alcove and haulage way)*
- *Re-computation of radiation view factors for deforming heated room surfaces*

Structural Analysis Features:

- *Quasistatic analysis with 294698 nodes / 279537 elements*
- *Large deformation, large strain formulation*
- *Nonlinear MD and power law creep models for salt*
- *Volumetric compaction model for the crushed salt*
- *Contact surfaces defined to allow arbitrary roof, rib, and floor contact*
- *Temperature dependent material properties*

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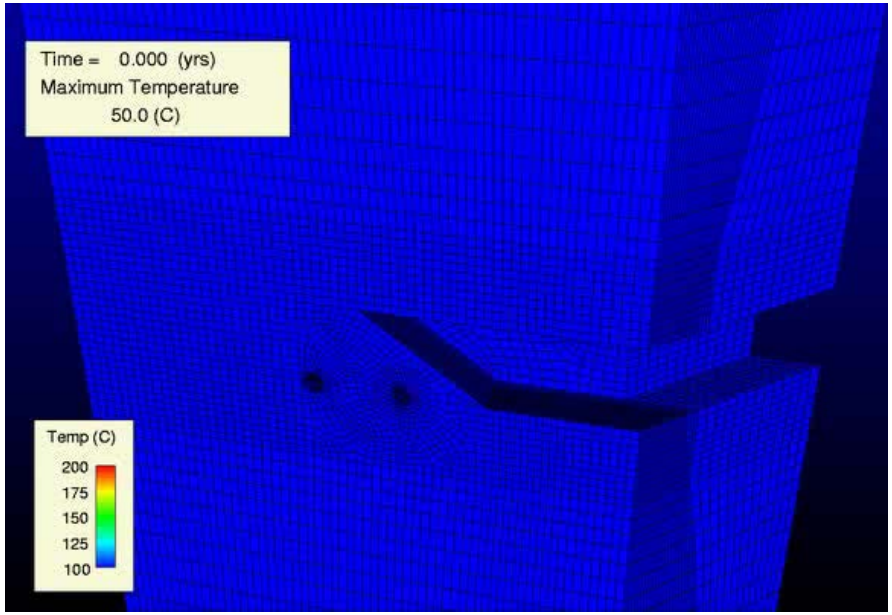
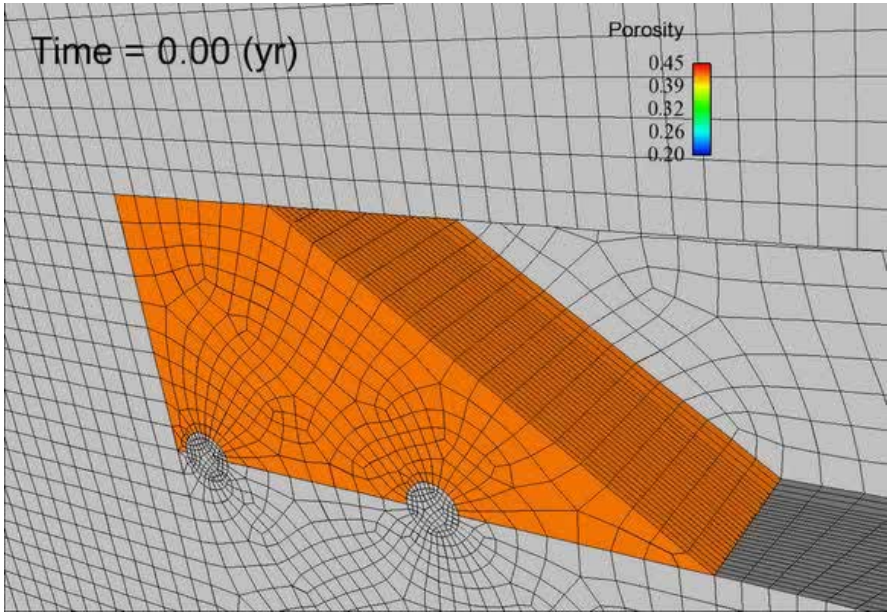
Closing Remarks and Observations on GSR

- *Computational effort is in contact algorithm and integration of constitutive models*
- *Full MD model is more expensive than the PLC by a factor of 3 (using 2nd mechanism of the MD only for the PLC)*
- *Stand alone PLC model in Adagio is 3 times slower than using the 2nd mechanism in the MD model to represent PLC behavior (difference due to method of integration)*



Repository Temperature Contours



Crushed Salt Backfill Porosity Contours

[Stone, C.M., Holland, J.F., Bean, J.E., & Argüello, J.G. 2010. Coupled Thermal- Mechanical Analyses of a Generic Salt Repository for High-Level Waste (ARMA-10-180). *Proc. American Rock Mechanics Association (ARMA) 44th US Rock Mechanics Symposium, 27-30 June 2010.* Salt Lake City: American Rock Mechanics Association.]

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Summary & Conclusions

- Have made some significant strides in adapting SIERRA Mechanics for repository applications
- A basic multi-physics capability has been demonstrated and is available in SIERRA Mechanics, but significant work remains to make it more general and accessible in a “production” capability sense
- Have done some preliminary validation of SIERRA Mechanics to ensure its applicability to repository problems; more needed, particularly for non-salt
- Continue to work on providing state-of-the-art “leading-edge” constitutive models for use in repository applications
- International collaborations are very important and are allowing us to leverage against many on-going efforts
- Testing and modeling of WIPP salt performed by German research groups is of enormous value to generic salt repository science

Questions??