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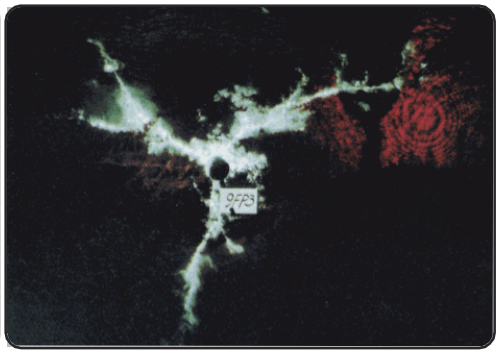


PFLOTRAN Model Development for Salt

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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PFLOTRAN

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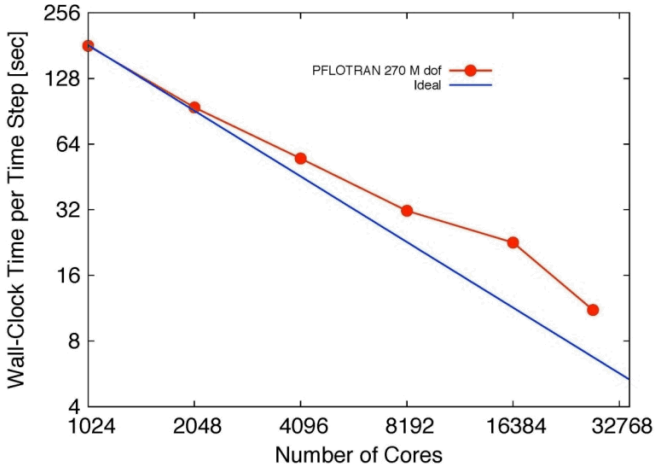
- **Petascale reactive multiphase flow and transport**
  - **Massively parallel**
  - **Process models important for salt**
    - Liquid and gas phase flow
    - Thermal convection and conduction
    - Multicomponent chemical reaction
- **Open source (GNU LGPL 2.0)**
- **Modern Fortran**
  - **Object-oriented Fortran 2003/2008**
- **Built on PETSc parallel framework from Argonne**
- **Demonstrated performance**
  - **Maximum # processor cores: 262,144 (Jaguar supercomputer at Oak Ridge)**
  - **Maximum problem size: 3.34 billion unknowns**



PFLOTRAN Multi-Physics Capability

- **Flow**
  - **Single phase, variably-saturated**
  - **Multiphase gas-liquid**
  - **Interchangeable constitutive models and equations of state**
- **Energy**
  - **Thermal conduction and convection**
- **Multi-Component Transport**
  - **Advection**
  - **Hydrodynamic dispersion**
- **Chemical Reaction**
  - **Aqueous speciation**
    - Ion activity models
  - **Mineral precipitation-dissolution**
  - **Sorption**
    - Isotherm-based
    - Ion exchange
    - Surface complexation
      - Equilibrium
      - Kinetic / multirate kinetic
  - **Microbiological**
    - Biomass
    - Inhibition
  - **Radioactive decay with daughter products**

PFLOTRAN for WIPP PA

- **Existing Legacy PA**
  - **Multiple 2D flow & transport models loosely coupled**
  - **Parallelized across multiple serial realizations only**
- **Switching to PFLOTRAN**
  - **Single 3D model can include everything**
    - {BRAGFLO, NUTS, DBR, MODFLOW, SECOTP2D} => PFLOTRAN
  - **Parallelize individual realizations**