Open-Source Software for Interfacing and Support of Large-scale Embedded Nonlinear Optimization

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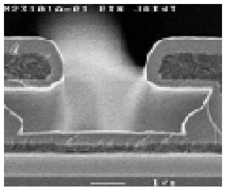
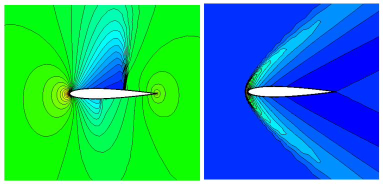
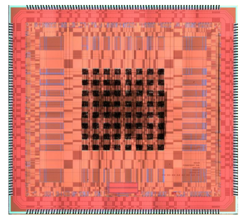
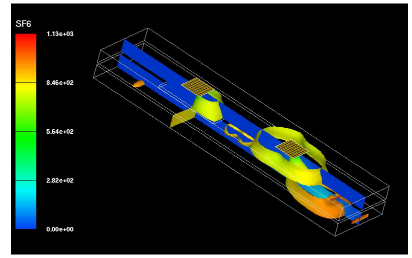
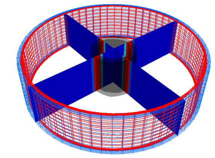
Computational Sciences at Sandia : PDEs and More …

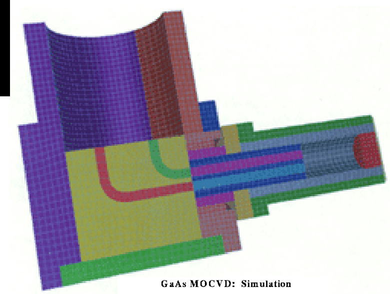


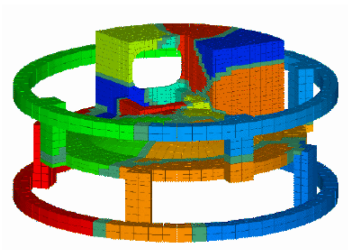




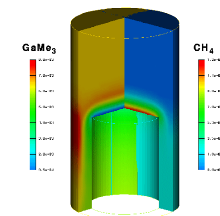


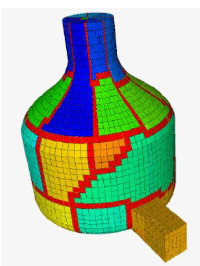


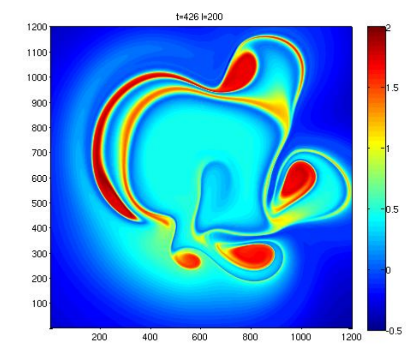




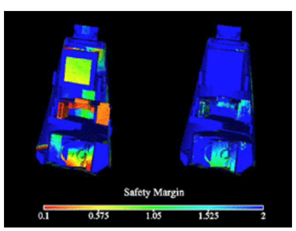
- Chemically reacting flows
- Climate modeling
- Combustion
- Compressible flows
- Computational biology
- Circuit modeling
- Inhomogeneous fluids
- Materials modeling
- MEMS modeling
- Seismic imaging
- Shock and multiphysics
- Structural dynamics
- Heat transfer
- Network modeling

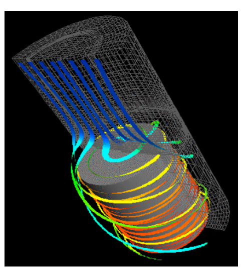


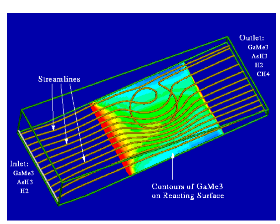


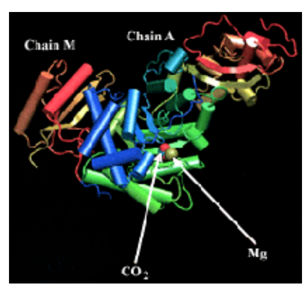


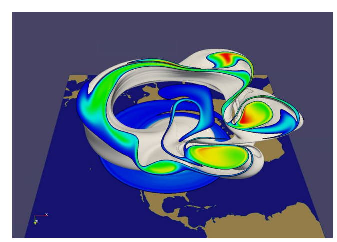
Large-Scale Parallel Distributed Memory and Implicit Iterative Solvers are Major Themes!











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Overview of Trilinos

- Provides a suite of numerical solvers to support predictive simulation for Sandia's customers

  => Scope has expended to include discretizations methods, …
- Provides a decoupled and scalable development environment to allow for algorithmic research and production capabilities => "Packages"
- Mostly C++ with some C, Fortran, Python …
- Advanced object-oriented and generic C++ …
- Freely available under and open-source LGPL license ...

Current Status

- Current Release Trilinos 9.0 (September 2008)
- Next Release Trilinos 10.0? (March 2009?)

Trilinos website

http://trilinos.sandia.gov

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Introducing Abstract Numerical Algorithms

What is an abstract numerical algorithm (ANA)?

An ANA is a numerical algorithm that can be expressed abstractly solely in terms of vectors, vector spaces, linear operators, and other abstractions built on top of these without general direct data access or any general assumptions about data locality

Key Points

- ANAs can be very mathematically sophisticated!
- ANAs can be extremely reusable!
- Flexibility needed to achieve high performance!

Example : Linear Conjugate Gradients

Given:

$A \in \mathcal{X} \rightarrow \mathcal{X}$: s.p.d. linear operator

$b \in \mathcal{X}$: right hand side vector

Find vector $x \in \mathcal{X}$ that solves $Ax = b$

Linear Conjugate Gradient Algorithm

Compute $r^{(0)} = b - \boxed{Ax^{(0)}}$ for the initial guess $x^{(0)}$.

for $i = 1, 2, \ldots$

$\rho_{i-1} = \langle r^{(i-1)}, r^{(i-1)} \rangle$

$\beta_{i-1} = \rho_{i-1} / \rho_{i-2} \; (\beta_0 = 0)$

$p^{(i)} = r^{(i-1)} + \beta_{i-1} p^{(i-1)} \; (p^{(1)} = r^{(1)})$

$q^{(i)} = \boxed{Ap^{(i)}}$

$\gamma_i = \langle p^{(i)}, q^{(i)} \rangle$

$\alpha_i = \rho_{i-1} / \gamma_i$

$x^{(i)} = x^{(i-1)} + \alpha_i p^{(i)}$

$r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$

check convergence; continue if necessary

end

Types of operations	Types of objects
linear operator applications	Linear Operators • A
vector-vector operations	Vectors • r, x, p, q
Scalar operations	Scalars • ρ, β, γ, α
scalar product <x,y> defined by vector space	Vector spaces? • $\mathcal{X}$

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