Summary of Special Session for WG5:

Collaborative Software Systems and Models

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Scope of WG5: Computational environment and algorithms

Solid earth is a coupled system of various complex phenomena extending over a wide range of scale. To enable the simulation of such phenomena, large-scale parallel computations and visualization technologies are required in order to simulate complex solid earth processes and to visualise the large amount of data generated. A high performance computational infrastructure, which promotes collaborative work among the geoscientists, is required for advancing the research front. The Working Group 5 (Computational environment and algorithms) covers these topics emphasizing on the computational aspect for earthquake simulations.

This special session is consist of four keynote talks at Yayoi Kaikan, Tokyo and eight poster/demo presentations followed by a technical meeting for more detailed discussions at Hakone Highland Hotel, Hakone. In this session, the following topics are focused on:

1. Collaborative software systems
2. Strategies for multi-scale / multi-physics coupling
3. High performance computing
4. Visualization technologies

Collaborative software systems

Computational infrastructure to realize the collaborative work among the different types of researches in the earthquake simulation and the use of high performance computing applied to various physical models in the solid earth is discussed. GEMCI (USA), LSMearth (Australia) and GeoFEM (Japan) are the three activities to be presented. Element technologies evolved in these are also discussed from other points of view listed below.

Strategies for multi-scale / multi-physics coupling

Coupling strategies among the different scale and/or different physical models for earthquake simulations are discussed. Particularly, computational aspect of *couplers* is emphasized. A part of outcome of the ACES visitors program also appears i.e. LSMearth-GeoFEM coupling and LSMearth-EFGM coupling.

High performance computing

Linear equation solvers, computational-tuning and mesh adaptation methodologies for large-scale problems are explored to make the best use of high-end computers. Numerical results of various solid earth simulations such as the outer core flow and the earthquake wave propagation are also presented.

Visualization technologies

The simulation of earthquakes requires complex visualization techniques in order to manipulate large-scale and long-history datasets. Applications of multidimensional wavelets and scalar field topology analysis presented here are the two approaches for this purpose. Parallelization of various rendering functions and related issues are also discussed.

Working Group

Introduction

We devoted a productive session on Thursday Oct 19 2000 at the ACES conference in Hakone Japan to setting up the computational environments and algorithms working group. The result of this meeting is described here. First we proposed as the initial vision: Identify, promote and establish computational techniques, environments and infrastructure to enable international collaboration to advance research and education in earthquake science.

Goals of ACES Working Group 5

- Establish cross working group standard Challenge problems and datasets
- List, organize and exchange software, algorithms and data
- Promote the standards and best practice methodology to ensure that software and data can be coupled together in multi-disciplinary applications and can run on the major machines of the ACES participants

This includes parallelization and visualization approaches and (XML) data structure standards :

- Track technology and report to community
- Identify ways of reducing unnecessary duplication by enabling re-use and encouraging particular projects to address international requirements

- Establish Geoscience specific requirements of generic information technology/HPCC techniques like visualization, computer architecture etc.
- Establish information resource for articles and links of importance from inside and outside community (e.g. XML standards efforts in other fields)
- Develop education material of Geoscience specific information technology/computational science and promote use in universities, conference tutorials and public outreach

ACES Working Group 5 Process

- Set up basic organization in first two months aiming at major successes by time of next ACES meeting (18 months). Develop publishable results and significant education/web resources in next year.
- Agree on 5 sub-groups -- each with at least two coordinators spanning ACES countries.
- List initial expertise / relevant projects of WG5 participants
- Solicit industry participation -- Hitachi. NEC, IBM, SGI, Sun ….
- Identify joint projects (such as LSMearth/GeoFEM collaboration; benchmark GeoFEM on USA machines)
- Identify funding for WG5 activities

ACES Working Group 5 Subgroups

Here we list subgroups and initial coordinators:

(1) Challenge problems :	Fox and Okuda
(2) Visualization :	Yuen and Fujishiro
(3) Middleware, Coupling and Data Structures :	Parker and Iizuka
(4) Algorithms and Parallelization :	Place and Nakajima
(5) Education :	Kellogg and another coordinator (preferably from outside USA)

ACES Working Group 5 Near Term Activities

- Send around information (minutes of first meeting) about WG5 to ACES community to gather initial working group members and information about their expertise and (local) activities
- Develop a "request" for other ACES working groups to gather input for WG5 subgroups – especially focus on challenge problems defined below.
- Challenge problems e.g large parallel granular motion code (requires load balancing and complex strategies which have been developed by other communities)
  - Visualization
  - Coupling
- Identify possible near term successes (low hanging fruit) -- for instance
  - Benchmark "GeoFEM on ASCI" or "Virtual California on Earth Simulator"
  - Paper on "Visualization in Earth Science" (issues, tools, experience)
- Establish (distributed) web resource for WG5
  - JPL will initially coordinate this

- Special Issue of *Concurrency and Computation: Practice and Experience* (Wiley) of Conference (and perhaps other) papers aimed at Computer Science community. This will be coordinated with the general ACES publication plan and has same deadlines. In spite of the arcane title, this journal focuses on practical computer science or computational science. Articles whose message is mainly the computational or numerical method or issues are suitable. Authors are encouraged to include geoscience background and results to provide context and requirements.
  - Submitted papers due end of January 2001
  - Final papers due May 2001
  - Publish September 2001
  - Hope to have strong representation from GeoFEM group but also papers from full ACES community

WG5 Participants: Interests and Subgroups

Here we list people, some of their interests and the subgroups with which they could be associated. This only lists people who attended the Thursday meeting and others will be added :

Geoffrey Fox Education, middleware, parallel algorithms; 2 3 4 5
David Yuen visualization and algorithms, molecular dynamics, CFD, Education ;2 5
David Place QUAKES, LSM/DEM, Visualization, object methods ;1,2,3,4
Peter Mora Micro/macro simulation/ACES Ex-officio
David Sparks granular physics, DEM, CFD, Education (earthquakes liked by public) ;5
Jay Parker GPS, quasistatic VE model,assimilation,;1,3,4
Gerald Hofer LSM, parallelisation, visualization ; 2,4
Steffen Abe LSM, gouge dynamics, friction laws, Object methods, parallelization ;4
Kengo Nakajima GeoFEM, linear solver/adaptation, Preconditioners, boundary element and FEM methods ;1,3,4
Yoshitaka Wada GeoFEM, mesh generation/pre-processing FEM;3
Hiroshi Okuda GeoFEM, Leader, Parallel FEM, CFD, meshless methods, middleware enabling interoperability ; 1 3 4 5
Kazuro Hirahara GeoFEM earthquake cycle model, propagation ;3
Hiroaki Matsui GeoFEM, Earth's core dynamics, MHD ;1,4
Mikio Iizuka GeoFEM, nonlinear, FEM and Finite difference CFD, coupling (LSMearth GeoFEM) ;3,4
Li Chen GeoFEM, visualization (parallelization, computer graphics) ; 2
Issei Fujishiro GeoFEM, Visualization (architecture, representation of complex fields, interactive design) ;2
Kazuo Minami GeoFEM, Performance Optimization/Solver ;1
Hisashi Nakamura GeoFEM,CES (Computational Earth Science) Director, does climate as well ;5
Kazuteru Garatani GeoFEM, static/dynamic solid mechanics ;1,4
Hideki Matsumoto NEC-RVSLIB, Visualization
Osamu Hazama GeoFEM parttime student, exchange with QUAKES on LSMearth-GeoFEM coupling, meshfree methods, parallelization