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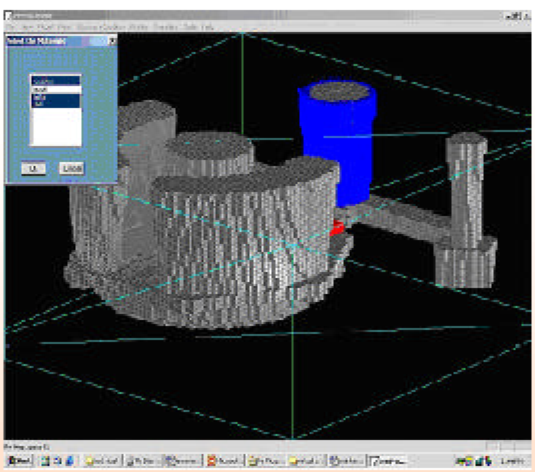
CSIR Network Projects on
Mathematical Modelling and Computer Simulation

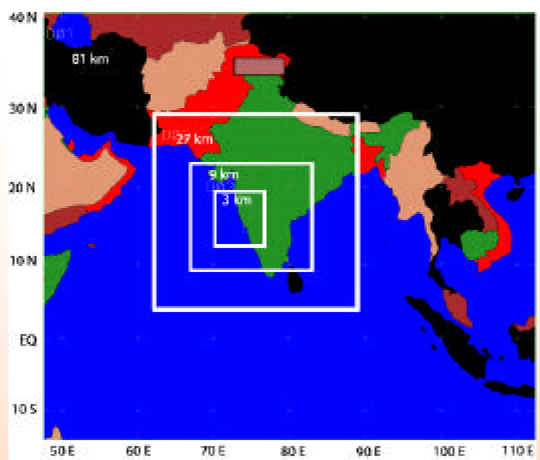
One of the greatest strengths of CSIR is its huge multi-disciplinary knowledge base, allowing limitless possibilities for synergy. The CSIR Network Projects were mooted to catalyze and promote such a synergy among various CSIR laboratories. The CSIR Network Project on Mathematical Modelling and Computer Simulation has been initiated to bring together expertise at a number of CSIR laboratories to foster and accelerate in a number of critical areas.. The use of mathematical and computational methods can now enlarge the range of scientific exploration to scales one cannot achieve otherwise even with the best instrumentation techniques available. The present project focuses on two major areas: High Performance Structures and Materials and Multi-Scale Environmental Modelling.

Highlights:

The year 2004-2005, the first year of the project, has seen the development of a closely knit group in the two areas of the sub-task. Under the sub-task I, the FINEARTS package involving finite element analysis has been calibrated and installed at the participant laboratories. Under Sub-Task II, a multi-scale environmental modelling platform has been now configured with a hierarchical organization of models.



Meshing using Virtual Casting Software



Domains of model integration with mutiple nests

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Sub Task I : Computational Mechanics for Modelling, Analysis and Design of High Performance Structures, Materials and Process Applications

Nodal Laboratory: SERC, Chennai, Co-ordinator, Dr N R Iyer

Participating Labs:

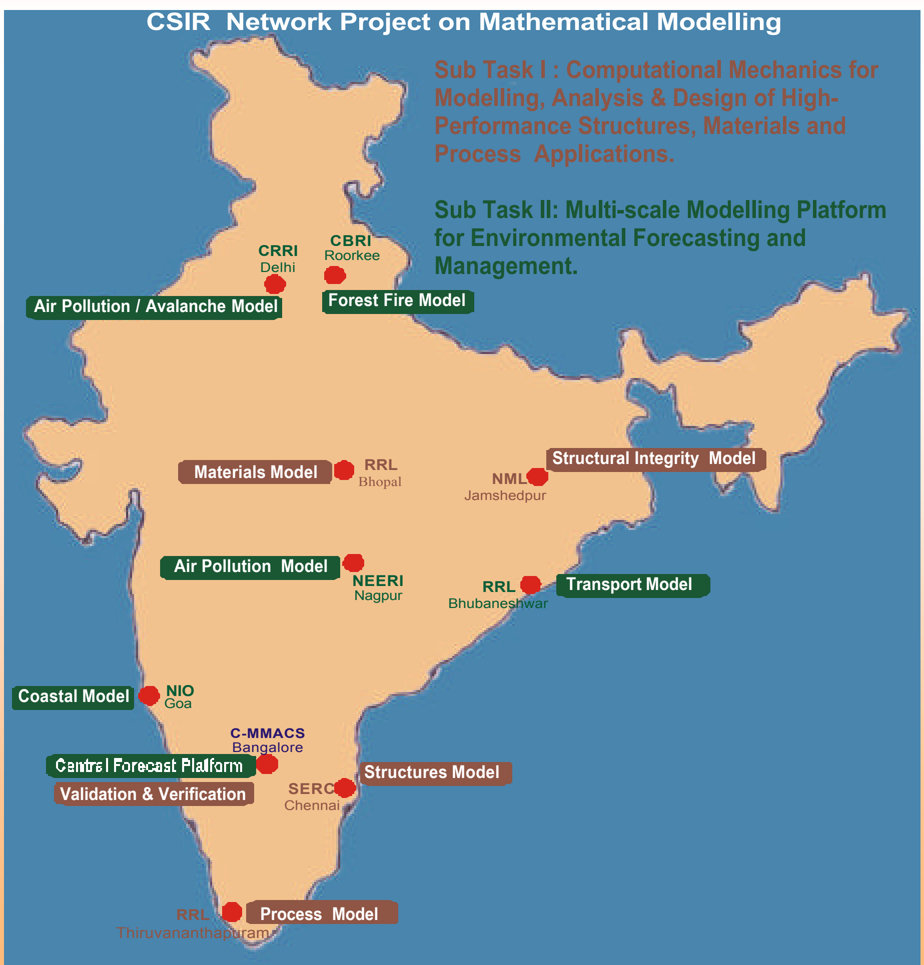
1. *CSIR Centre for Mathematical Modelling and Computer Simulation, Bangalore (C-MMACS)*
2. *Regional Research Laboratory, Bhopal (RRL-Bho)*
3. *Structural Engineering Research Centre, Chennai (SERC)*
4. *Regional Research Laboratory, Trivandrum (RRL-Tvm)*
5. *National Metallurgical Laboratory, Jamshedpur (NML)*

Sub Task II : Multi-scale Modelling Platform for Environmental Forecasting

Nodal Laboratory: C-MMACS, Bangalore, Co-ordinator, Dr P Goswami

Participating Labs:

1. *CSIR Centre for Mathematical Modelling and Computer Simulation, Bangalore (C-MMACS)*
2. *Central Building Research Institute, Roorkee (CBRI)*
3. *Central Road Research Institute, New Delhi (CRRI)*
4. *National Environmental Engineering Research Institute, Nagpur (NEERI)*
5. *National Institute of Oceanography, Goa (NIO)*
6. *Regional Research Laboratory, Bhubaneswar (RRL-Bhu)*



4.1 Sub Task I : Computational Mechanics for Modelling, Analysis and Design of High Performance Structures, Materials and Process Applications

The activities of the project under sub-task II have been worked out in detail towards achieving the envisaged objectives of the project. It has been planned to develop an indigenous Finite Element (FE) software package which could be a viable alternative for the existing commercial FE packages. As a base line of the software development exercise, a research code FINEART [FINite Element Analysis of structures using Adaptive Refinement Techniques] on Linux platform developed by SERC has been identified. A familiarization programme on FINEART 3.0a was conducted. The aim of the programme was to impart working knowledge of the software so that further development could be integrated with the software in addition to its validation and verification.

SERC reorganized FINEART (ver.3.0a) to take care of the following aspects:

- Easy implementation of additional finite elements
- Adding new material models
- Adding analysis features (linear & non-linear dynamics)
- Solving very large size problems (few million dof)
- Interfacing with commercial FEA software

The modules related to memory allocation have been completely reorganized by replacing the blank common with dynamic memory allocation of arrays. The reorganized FINEART program has been successfully tested for standard static problems. Work towards integrating the existing sparse solver with the reorganized FINEART has been taken up. A number of benchmark and validation studies were conducted by C-MMACS to check the performance of 4-noded, 8-noded and 9-noded plane stress/strain and plate/shell elements available in FINEART. From the studies, it is observed that the 4-noded (QUAD4) plate/shell element failed in some test cases. To improve the performance of this element, 4-noded edge consistent plate bending formulation for QUAD4 element has been successfully implemented. Number of example problems solved using this element showed remarkable improvement in the performance.

4.1.1 Development of Smart Structure Module in FINEART Program, C-MMACS

A program module for computation of stiffness matrix for laminated composite beam element based on first order shear deformation theory has been developed at C-MMACS. Work towards implementation/integration of this module in FINEART program is under progress. For the development of smart structure module in FINEART, preliminary studies were carried out at C-MMACS. The development of piezoelectric beam element has been taken up. Few a posteriori error estimators for nonlinear problems have been identified and an independent module has been implemented for one-dimensional problems. Necessary tests are being conducted. The formulation of error estimators will be extended for plane stress/strain problems.

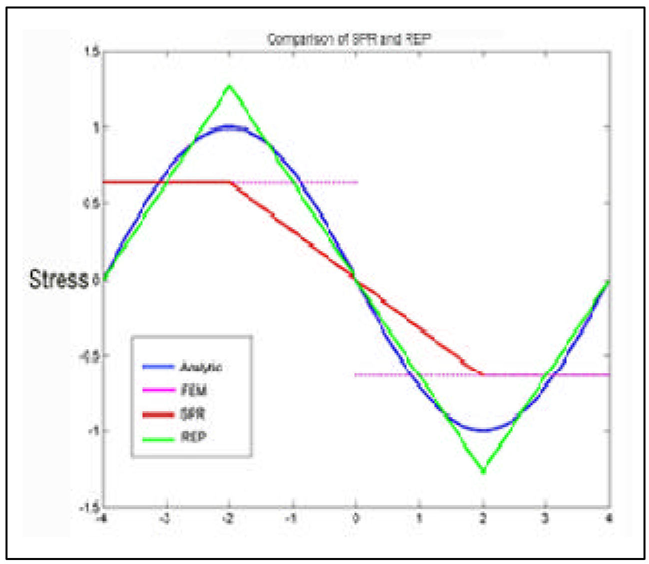


Fig 4.1 Comparison of stresses recovered between Superconvergent Patch Recovery and Recovery by Equilibrium in Patches.

Adaptive mesh-refinement techniques based on a *posteriori error* estimators have become as indispensable tool in large scale scientific computing. FINEART uses superconvergent patch recovery technique to compute the error estimates and the h-refinement adaptive process is implemented based on bi-section for mesh-refinement. The objective is to formulate an a *posteriori error* estimator for 4-noded plane stress strain element considering geometric nonlinearity.

For nonlinear problems, it is shown that the accuracy and stability of superconvergent patch recovery (SPR) method can be remarkably improved through (i) use of integration points as sampling points, (ii) weighted average procedure and (iii) introduction of additional nodes. Another super-convergent method known as Recovery by Equilibrium in Patches (REP) does not need any knowledge of superconvergent points and is consistent with nonlinear formulations too. It is based on equilibrating the recovered stresses, in the patch. The stresses recovered by this method have been compared with the SPR methods for a 1-D problem (Fig 4.1). Recently, another method based on Variation Mapping Functions and error distribution (VMF) has been proposed. Taking the variation of the error energy about the mapping function tractions are recovered on the element interface. To understand the characteristics of the proposed error estimator a one dimensional problem has been analyzed by the above method.

4.1.2 Structural Engineering Research Centre (SERC), Chennai

SERC updated the FRACANA module of for fracture analysis FINEART with MVCCI (Modified Virtual Crack Closure Integral) and J-integral technique in addition to displacement extrapolation technique. These modules have been integrated with FINEART. Validation studies on fracture analysis of a plate with centre crack and edge crack have been carried out by employing 4-noded, 8-noded employing 4-noded, 8-noded (regular and singular)

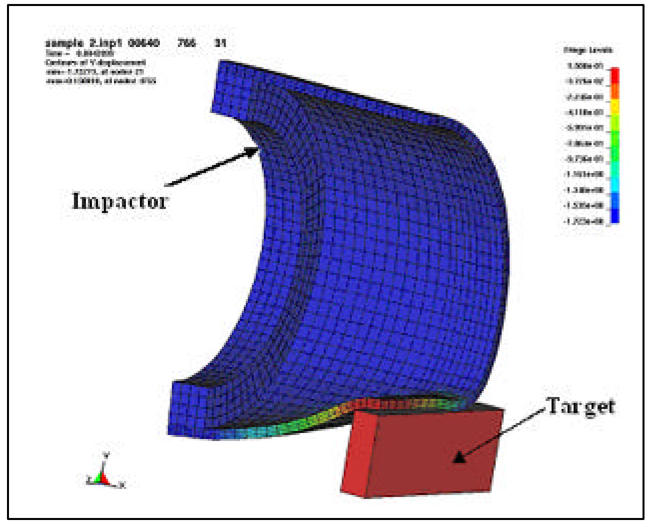


Fig 4.2a Deformation in Y-Direction at t = 0.035 s

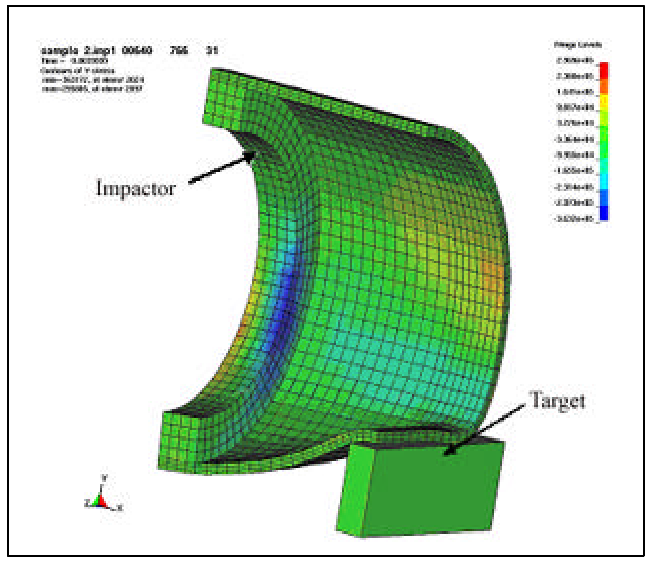


Fig 4.2b σ_{yy} (max) stress at t = 0.0035 s

and 9-noded plain stress elements. The stress intensity factors obtained in the present study by using displacement extrapolation, MVCCI and J-integral techniques have been found to be in close agreement with the analytical solutions. A public

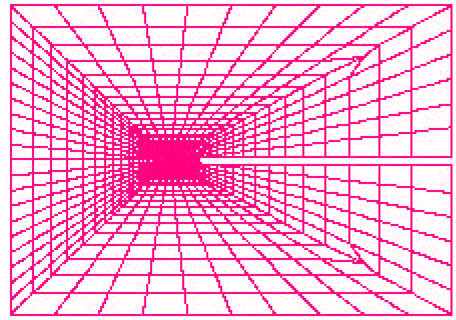
Table 4.1 Result of the studies of the impact of a cylinder on to a rail.

Impactor		**Details**	**Impactor**	**Target**
Material	Steel	G (psi)	$1.133x10^7$	Rigid
Dia. of Cylinder	9 in.	K (psi)	$2.4x10^7$	Rigid
Length	12 in.	σ_y (psi)	$1.9x10^5$	Rigid
Thickness	0.25 in.	Density ($lb\text{-}s^2/in^4$)	$7.35x10^{-4}$	$1.47x10^{-2}$
Initial velocity	660 in/sec.	E (psi)	N/A	$6x10^7$
Sliding Interface	**Rigid wall interface**	**Material model**	Isotropic	Elasto-plastic

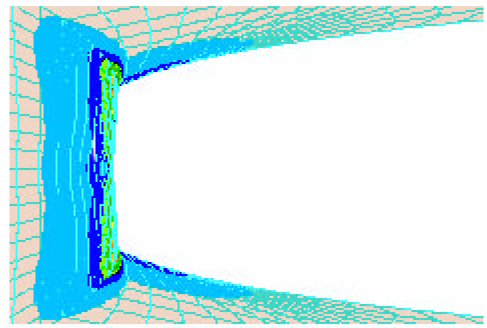
domain software which is useful for non - linear explicit transient dynamic and impact with different sliding interfaces. Various analysis has been implemented by SERC. This software has the capability to analyze large structures for complex loadings such as impulse material models to represent the material behaviour in linear and non-linear analysis have been made available. Some of the commonly used material models such as "elastic" and "isotropic-elastic/plastic" have been tested. Studies of the impact of a cylinder on to a rail have shown excellent performance (Table 4.1 and Figs 4.2a and 4.2b).

4.1.3 Regional Research Laboratory (RRL), Bhopal

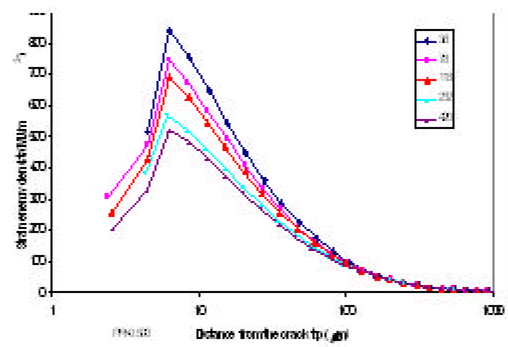
During the strategy planning by RRL, Bhopal after consultations, it was decided to have an independent solver for metal forming and integration of this with FINEART through pre- and post processors. Both the solvers will be integrated through single pre and post processors. Pre- and post processing commands required for large plasticity software has been worked out. During this period, methodologies to develop large plasticity module, was attempted. Simulations of standard problems were carried out using commercial FE software that includes elastic as well as large deformation plasticity problems. The results were validated with reported experimental and analytical results. It was found that these are quite close. Large plasticity simulations have been carried out using the RRLFEM software which works on total elastic incremental plastic formulation. Simulated metal forming, dislocation and fracture mechanics problems have been successfully conducted. Ductile fracture analysis of CT specimen were carried out considering macro, meso and micro scales. It was found that results are in good agreement with the experimental results.



a. Initial mesh



b. Crack tip



c. Distribution of strain energy

Fig 4.3 show the results for the ductile fracture of a CT specimen.

Table 4.2 Comparison of various methods

Grain size (mm)	1/sqt (grain size)	J (kJ/m^2) (exp)	micro J (kJ/m^2) (SZW)	macro J (kJ/m^2)(load disp)	meso J (kJ/m^2) (path indep)
38	0.1622214	190	180	211	175
78	0.1132277	170	165	183	161
118	0.0920575	140	159	170	143
252	0.0629941	120	142	147	133
420	0.048795	93	136	140	126

4.1.4 Regional Research Laboratory (RRL), Thiruvananthapuram

Strategy and planning for GUI towards enhancing the features of pre-processor to FINEART has been worked out by RRL, Thiruvananthapuram in consultation with SERC. RRL-Thiruvananthapuram has been developing an FDM based casting simulation package called Virtual Casting (Fig 4.4).

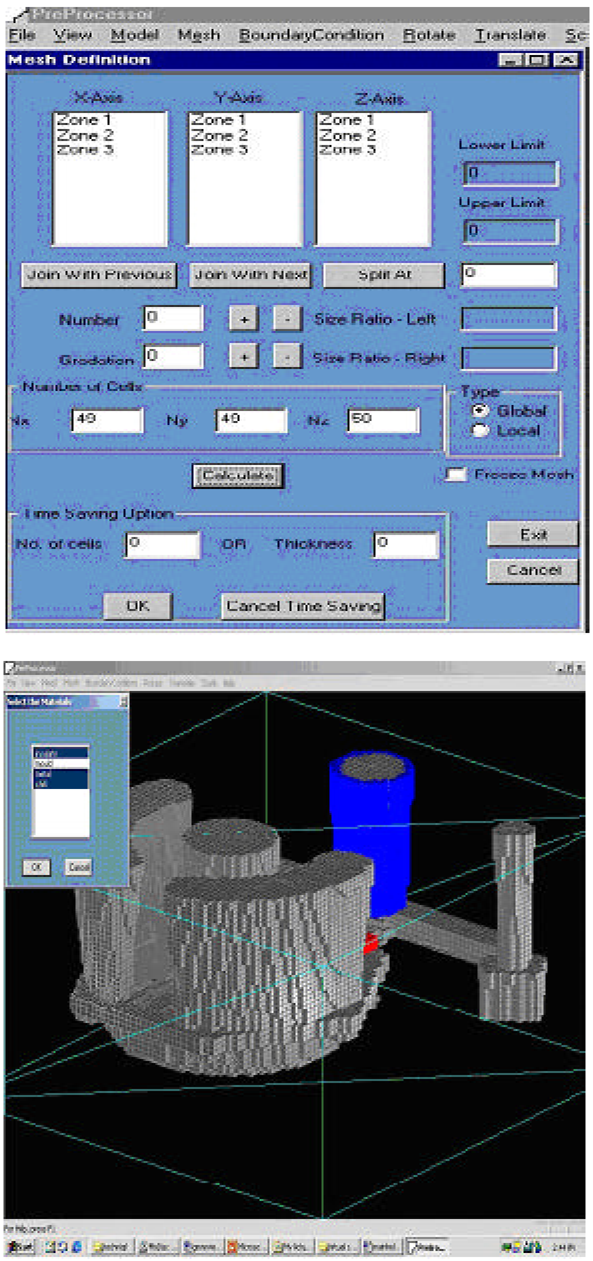


Fig 4.4 Meshing using Virtual Casting Software.

The package is being upgraded - converted to FEM and new features added - by integration with FINEART. Meanwhile the original package has been brought into the market. Two licenses have been transferred to Indian Institute of Foundary R&D Center in Hyderabad and a validation exercise has been initiated involving foundry clusters in Hyderabad and Vijayawada. The solution of the governing equations is being re-formulated using FEM. During the next quarter this will be intergrated into FINEART. A tentative design has been made for the graphical user interface for the whole package keeping in mind the requirement of modularity for the different packages which are going to be integrated with FINEART. Literature is being studied to arrive at an appropriate meshing algorithm that will create an FEM mesh on 3D geometry models created using any standard CAD software.

4.1.5 National Metallurgical Laboratory (NML), Jamshedpur

Literature review on the elasto-plastic concepts of fracture mechanics has been carried out by NML-Jamshedpur. NML got familiarized with the software package FINEART and also carried out literature review on elasto-plastic concepts of fracture mechanics. In addition, finite element (FE) analysis has been conducted using standard fracture mechanics specimen using commercial software package, to investigate the elastic-plastic stress fields near the crack tip. The extent of deformation at the crack tip was estimated through quantitative fractography by measuring stretch zone dimensions. FE results have been verified with the same obtained experimentally. A good agreement was found in elastic region, however, in non-linear region, the numerical results differ with the experiments. The probable causes identified were non-availability of sensors for measuring crack growth with a precision of 20 micron and the inherent errors in the FE solver of used for the computation.

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4.2 Sub Task II Multi-scale Modelling Platform for Environmental Forecasting and Management

Accurate assessment and advance warning of environmental processes like air pollution, land-slide, forest-fire and fog can significantly improve our approach to manage related hazards. This requires a comprehensive multi-scale modelling of these systems based on sound physical and mathematical principles.

The basic modelling strategy adopted for Sub-task II is to use an organized hierarchy of models to simulate environmental processes at different scales. At the heart of the modelling platform is a meso-scale model that describes three dimensional dynamics of atmospheric circulations, driven by boundary forcing and moist processes. The output from this model such as wind, temperature and rain then provide inputs to various process models like air pollution, landslide and forest fire. A schematic representation of the proposed multi-scale modeling platform is given in Fig 4.5.

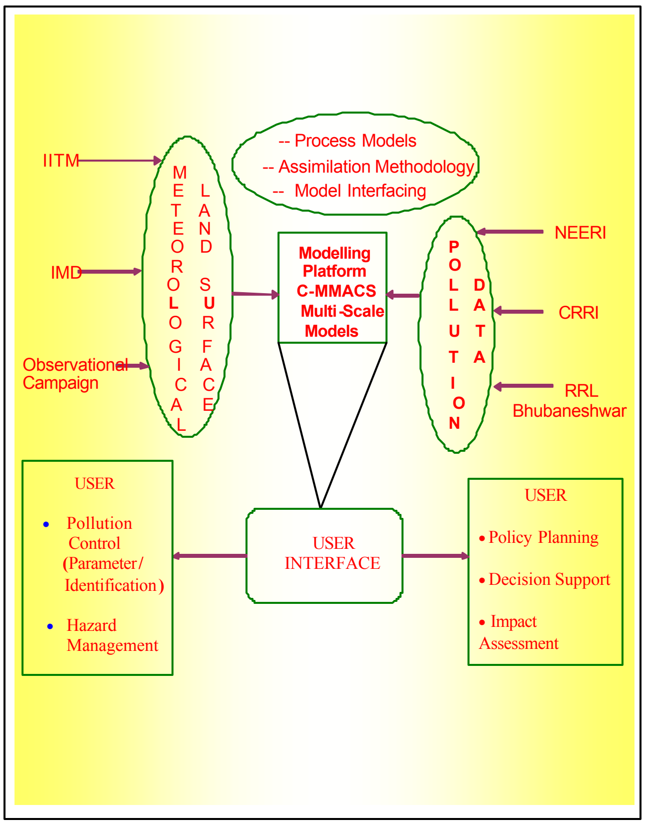

Fig 4.5 A schematic representation of multi-scale environmental modelling platform

The strategy is to develop components and databases at different participating laboratories. The components first developed and calibrated in stand-alone mode are then integrated into the multi-scale modelling platform. The integrated platform is further calibrated and validated against observed data.

4.2.1 Installation and Calibration of MM5, C-MMACS

The meso-scale model that generates grid-point, multi-level data for different dynamic and thermodynamic variables is the driving engine for the multi-scale modeling platform. We have adopted the Version 3.5 of the model MM5 as the primary candidate for the meso-scale model. This model has been now installed at C-MMACS computing platform, configured and calibrated for a number of forecast configurations.

In particular, the model has been configured to generate simulation with resolution upto 1 km over a given domain. At the same time, extensive simulations experiments were carried out to determine optimal configurations for simulations at different (meso) scales.

As is well known, the quality of simulations strongly depends on the choice of the parameterization schemes. The choice of parameterization schemes, however, depends on the scale of the process and resolution of the process. An important part of the model calibration is therefore choice of optimum parameterization schemes. A series of simulations was carried out to assess relative merits of different parameterization schemes for monsoonal convective systems, taking advantage of multiple choices available in MM5.

Simulation of a Heavy Rainfall Event: A series of simulations were carried out for a heavy rainfall event that occurred along the west coast of India during monsoon on 13 June 1988. The model was set up with 4 nested domains 81 km, 27 km, 9 km and 3 km grid spacing with 23 vertical levels; Fig 4.6 shows the domains of integrations, with the four nests with their respective resolution.

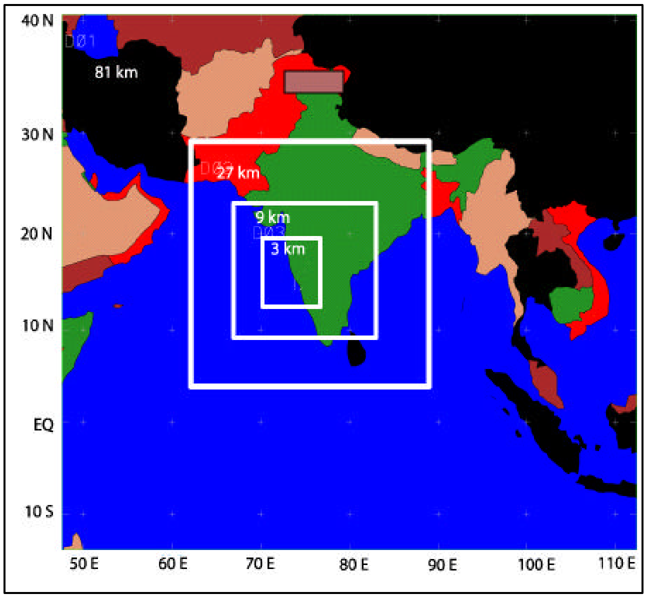

Fig 4.6 Domains of model integration with mutiple nests.

The model was initialized at 00z 11 June 1988 using the NCEP's 2.5 degree girdded analysis. We have carried out the simulation with different cumulus parameterization schemes such as Anthes-Kuo, Betts-Miller, Grell and Kain-Fritch schemes. We have kept the boundary layer

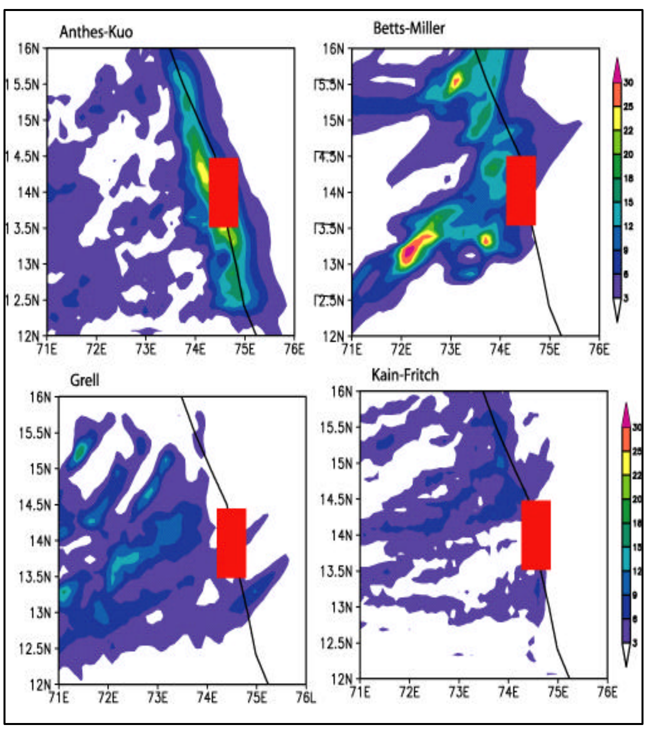

Fig 4.7 Simulated 24 hour rainfall for different parameterization schemes. The area observed heavy rainfall is marked with the red square.

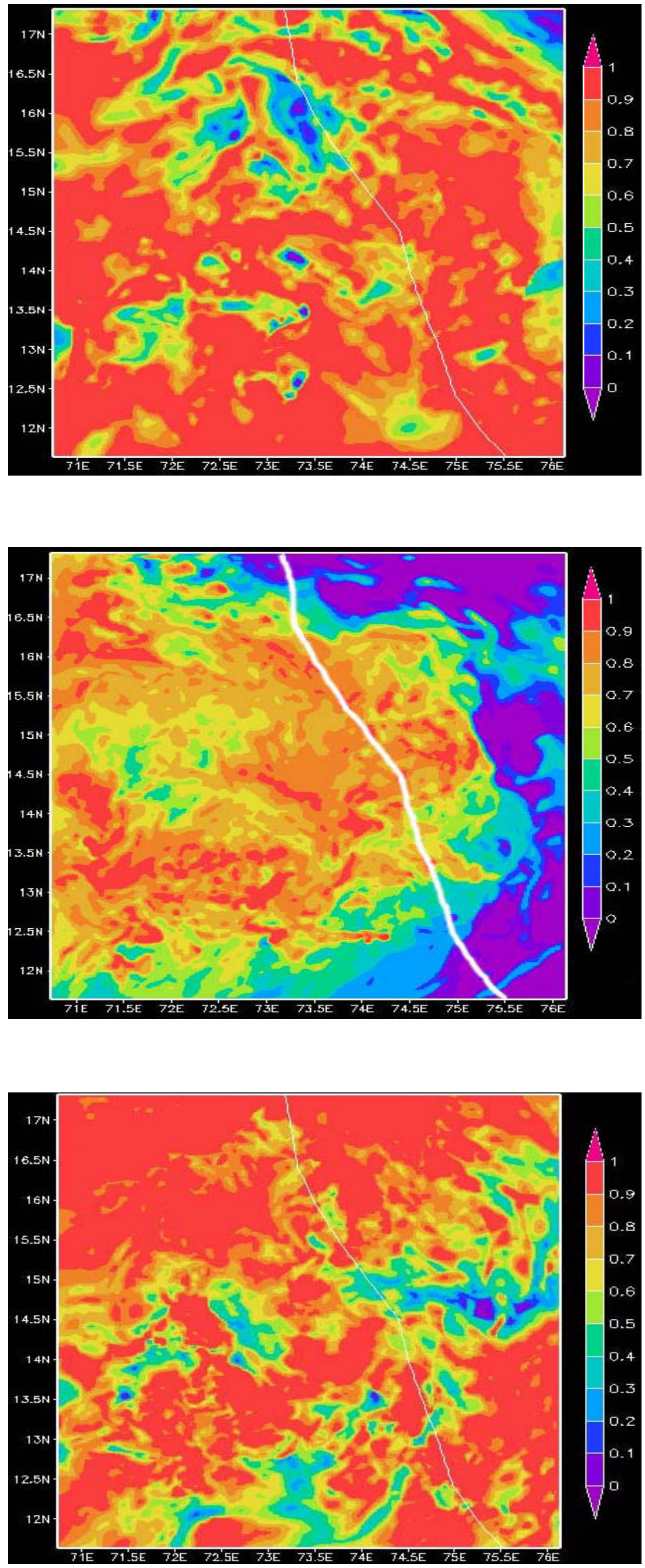

Fig 4.8 Longitude-latitude distribution of 24-hour cloud field of different vertical extent: high (top panel), medium (middle panel) and low (bottom panel) associated with a heavy rainfall event simulated with MM5.

scheme and Simple Ice microphysics for all simulations. The model was run for 48 hours and last 24 hour rainfall is shown in Fig 4.7. A scrutiny of Fig 4.7 reveals that while the Anthes-Kuo scheme gives less error in amount and position of rainfall, the Betts-Miller scheme gives better results in terms of the amount of rainfall, however the Betts-Miller scheme failed to capture position. The other two schemes failed in both amount and position. These simulations form a key component in calibrating and configuring the model for the monsoon region.

Cloud-scale Simulation: The MM5 model configuration was also tested for simulation of cloud field with a very high resolution in the inner most (of 5 nest) nest of 1 km. Fig 4.8 shows three different cloud fields: high, medium & low, in a 24 hour simulation over the west coast.

While such a simulation of a single event is at best only indicative of the model to resolve features of a complex process like a convective cloud; this prepares the background for a comprehensive statistical evaluation of the model skill at these scales.

Regional Scale Simulation: Sensitivity of Moist Processes to Vegetation: The land surface and bio-aspheric process are known to play important roles in convective dynamics that dominates the monsoon weather and climate. A series of simulations was carried out to examine and quantify the impact of vegetation data on moist processes over the monsoon domain.

Fig 4.9 shows the effect of different vegetation datasets on precipitation processes. Normalized contrast (between ISRO and Climatological Vegetation Fraction) in perceptible water varied between -6 to 5% respectively between two different vegetation data sets.

While these results on effect of vegetation on moist processes are only indicative at the moment owing to the small sample size, the broad conclusions are likely to be true in general. Thus, accurate vegetation data with its temporal variability appears

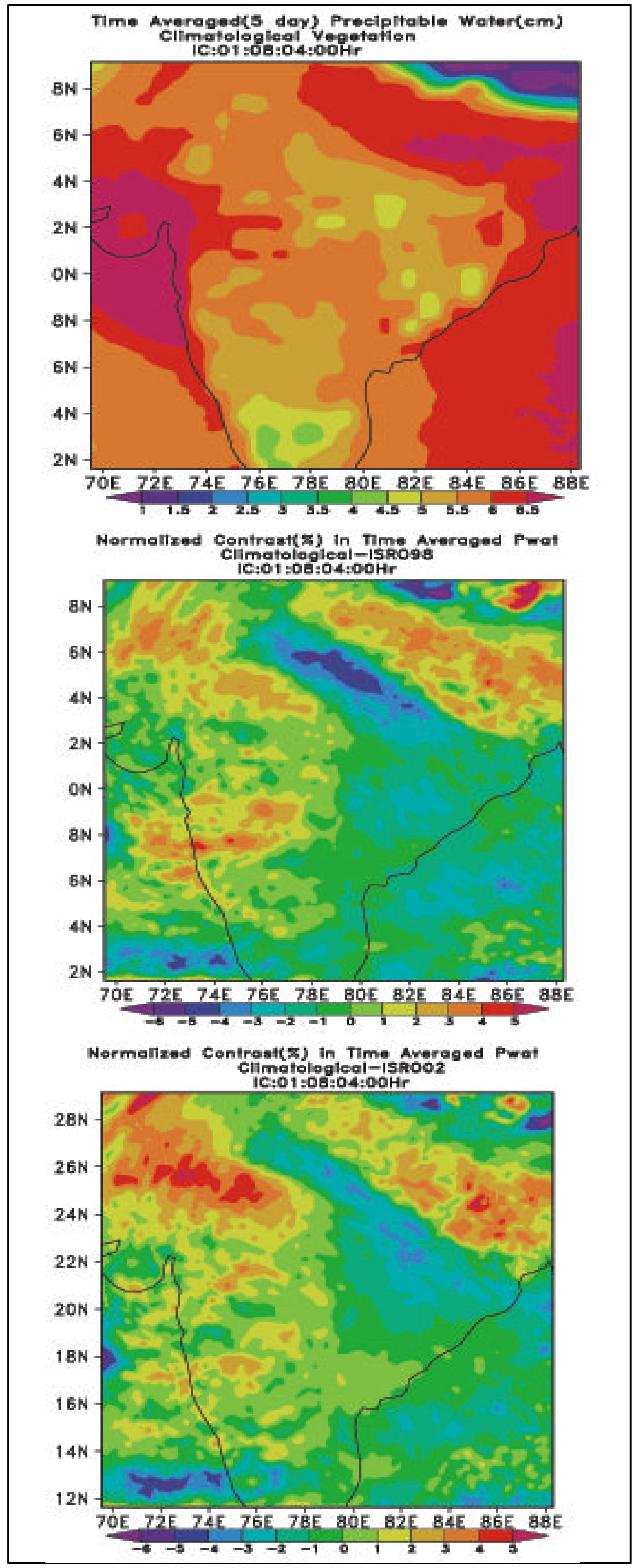

Fig 4.9 Lat-long Structure of Normalized Contrast (%) in Time Averaged Perceptable Water.

to be an important ingrediant even for short-term (a few days) evolution of moist processes. In other words, agricultural policy including crop choice and irrigation pattern are likely to play important roles in the evolutionn of local weather pattern.

These results indicate that a carefully calibrated and configured model can simulate many aspects of an extreme weather event like a heavy rainfall. At the same time the results highlight the need for a careful scale-specific model configuration with proper choice of parameterization schemes.

However, these simulations need to be evaluated against observations in a statistical sense.

4.2.2 Emission and Landslide Modelling, CRRI

Emission Modelling: The objective of this component is to develop a pollution profile (arising out of vehicular pollution) based on the primary and secondary data. Under this part of the project detailed project report has been prepared and submitted to CMMACS, Bangalore (the co-ordinating agency of CMM0020). Literature survey has been conducted on the existing model on emission and noise pollution. Based on this, a state of the art report has been compiled. Based on this technology scan various input parameters used in the management of urban air quality purposes have been identified. A study area and road network has been selected for the development and application of emission model. Development of the spread sheet to calculate the vehicular emission loads for the test case is in progress.

Landslide Hazard Modeling: The scope and objective of this part of the project is to formulate the guidelines for predicting rainfall induced landslides by analytical model under this part of the project, a detailed project report (DPR) has been prepared and submitted to CMMACS, Bangalore as in the first part.

a) Development of one dimensional model to simulate the suction and moisture content in a slope at different depths vertically downwards from the ground surface for different time intervals from the start of rainfall is in progress.

b)A two dimensional plane strain study of slope failure by simulating the soil as elasto-visco-plastic material with Mohr-Coulomb failure criterion and non-associated flow rule is in progress.

4.2.3 Air Pollution Modelling, NEERI

Development of GIS based Air Pollutant Transport Model for Urban Area: NEERI is engaged in developing emission and loss inventory models for air quality assessment based on regional meteorological model of CMMACS. While the inventory models are GIS based, taking geographical details from GIS and Remote Sensing Imageries on land use, the transport model for air quality modelling is based on Lagrangean Particle Tracking Random Walk technique.

Detailed, girdded emission inventories are required as input to air quality models and must include emissions estimates of pollutants reported at the grid-cell level. Modeling grids may extend over multi-scale domains and may include hundreds of grid cells, depending on grid resolution. For large point sources such as power plants and factories, geographic coordinates are commonly reported with emission or can be easily recorded with a GPS. Area sources like JJ Clusters where wood or coal burning emissions are considerable also need to be accommodated in the emission inventory.

Using Arc Macro Language (AML) programming, a software has been written for defining the grid system with any desired grid size over a digitized map of an urban area. The road network for line sources as well as other point and area sources are also digitized in separate coverages linked with the details of emission sources in Access database. The road information include the hourly traffic volume of different types of vehicles in different roads and emission rates for different pollutants emitting from different types of vehicles. Area sources are computed from per capita emission and population density of the clusters. Location specific point source data are obtained through their specific emission rates. GIS estimates grid wise total emission of different pollutants from all point, line and area sources for different hours. Based on the daily maximum and minimum values, appropriate color codes are generated for different emission levels of the grids and plotted for visualization.

Studies on Air Quality and Emission Inventory: For actual application, the city of Delhi has been chosen. The digitization of the city map is in progress. For model calibration, the vehicle counting and continuous ambient air quality measurement along with meteorological data collection programme have been taken up by NEERI for the Delhi city. Substantial past data is also available from different sources.

Ambient air quality in Delhi has been monitored by the National Environmental Engineering Research Institute (NEERI) as part of the National Air Quality Monitoring Network (NAQMN). Sulphur dioxide (SO_2), SPM and nitrogen dioxide (NO_2) have been measured at three sites between 1978 and 1987. Results were published in a series of Air Quality in Selected Cities reports. Annual mean airborne lead (Pb) concentrations were determined at the three NEERI sites in 1990. The Central Pollution Control Board (CPCB) commenced air quality monitoring at five stations in 1987; however, these results are not directly comparable with those from the NEERI sites because of differences in siting criteria and methodologies.

4.2.4 Atmospheric Transport Model, RRL

Several available atmospheric chemistry models have been studied viz. MATCH (Multiscale Atmospheric Transport and CHemistry model Swedish Meteorological and Hydrological Institute), ASAD (A Self-contained Atmospheric chemistry code), MATCH (A Model for Atmospheric Transport & CHemistry model developed by National Center for Atmospheric Research, Colorado) and WRF/CHEM as well as Chilean Air Pollution dispersion model (CADM).

The SMHI MATCH model is a Eulerian model and the meteorological data are taken from external sources or from dynamical weather forecast model. It can simulate transport, deposition and ASAD is basically an atmospheric chemistry module with a chemical reaction database and for apparent lack of conservation in SLT schemes. Because of its inherent drawback several corrective algorithms have been suggested.

WRF (Weather Research and Forecasting)/CHEM (chemistry) model developed by NOAA/FSL can be used for coupled weather/dispersion/air quality prediction. It has several modules integrated together such as dry deposition, biogenic emission, chemical mechanism, photolysis and aerosol.
The CADM uses the PSU-NCAR MM5, which provides the meteorological output such as time-dependent three-dimensional wind, temperature, pressure, and specific humidity and a chemistry-transport module (CTM) that uses the meteorological output to predict the time-varying trace gas concentrations by solving the species conservation equation.

Having studied the above models it was found that SMHI MATCH, WRF/CHEM model and CADM might be most suitable for the present study. It is proposed to modify these models as per the requirement and use it for prediction of pollutant concentration. Work on collection of data from various sources has been initiated. Air quality data has been collected from Orissa Pollution Control Board (OPCB) for the period January 2004 to September 2004 for 14 stations in Orissa located at Bhubaneswar, Cuttack, Rourkela, Balasore, Angul, Rayagada and Talcher. For most of the stations the data were collected twice weekly on 4 hourly basis i.e. six readings per day. The various parameters were SO_2, NO_x, SPM measured at a height of 20ft. Efforts have also been made to collect point source emission data for various industries in Orissa from OPCB. In addition daily analysis of rainwater during monsoons and weekly analysis of dry washings during dry seasons for cations such as Na^+, K^+, Ca^{2+}, NH^{4+} and anions such as Cl^-, SO_4^{2-}, NO_3^- have been carried out at one station in Bhubaneswar by RRL Bhubaneswar.

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