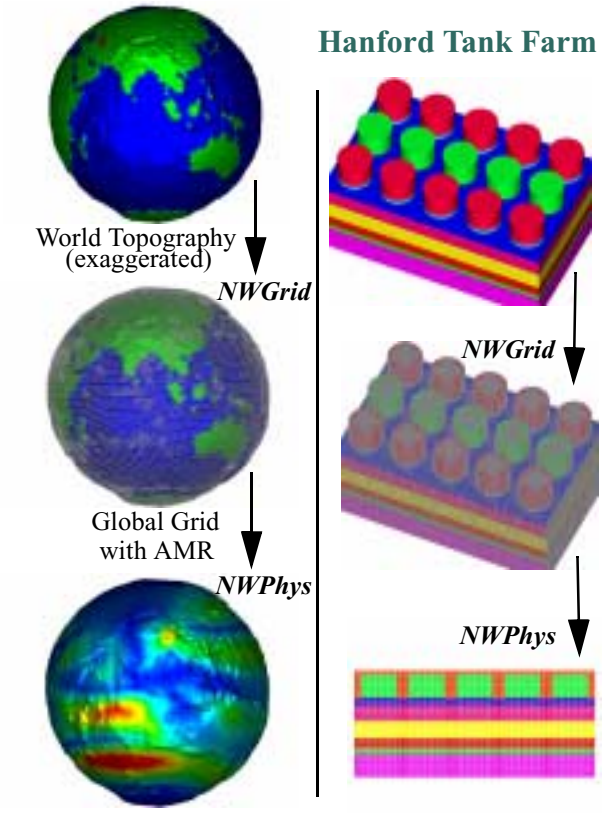
Ion Trap

Hanford Tank Farm



William R. Wiley
Environmental Molecular Sciences Laboratory

The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), the U.S. Department of Energy's (DOE) newest national scientific user facility is located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. The EMSL is operated by PNNL for the DOE Office of Biological and Environmental Research to facilitate multidisciplinary approaches to complex scientific and technical problems relevant to DOE missions and the nation's environmental challenges.

Capabilities in the EMSL include over 100 major instrument systems available to users, our resident research staff, and their collaborators. These capabilities are used to enable fundamental research on the physical, chemical, and biological processes that underpin critical environmental issues.

More information about EMSL capabilities and research programs is available on the EMSL web site.

http://www.emsl.pnl.gov

Staff members on the ***NWGrid/NWPhys*** team include:
Dr. Harold E. Trease
Lynn Trease

Applied Mathematics Group in the Theory, Modeling, and Simulation Directorate.

More information about ***NWGrid/NWPhys*** is available on the EMSL web site:

http://www.emsl.pnl.gov:2080/nwgrid
http://www.emsl.pnl.gov:2080/nwphys

For additional information about ***NWGrid/NWPhys***, please contact:

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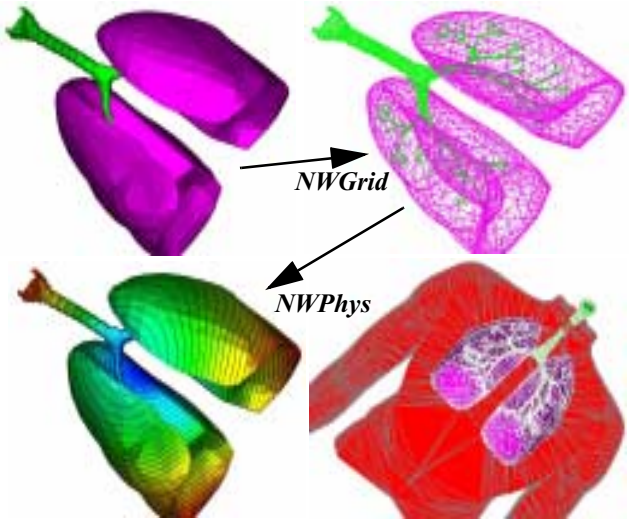
William R. Wiley
EMSL
Environmental Molecular Sciences Laboratory

NWGrid/NWPhys

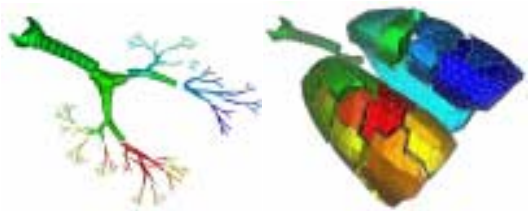
The *N*orth*W*est *Grid* Generation and *Phys*ics Codes



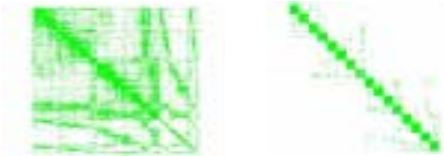
Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy

The Virtual Biology Center Lung Modeling

Parallel Processing



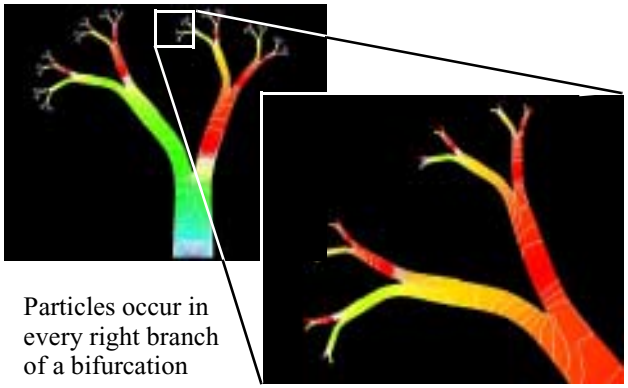
Unstructured, virtual lung mesh is partitioned and mapped to 16 processors, using METIS.



Graph of mesh connectivity BEFORE decomposition

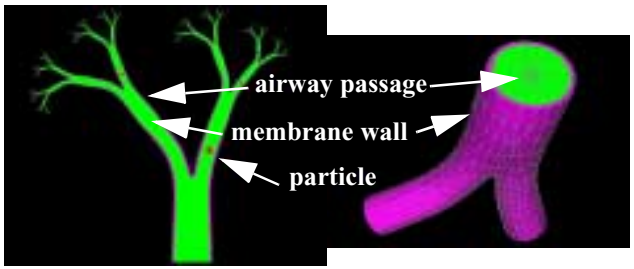
Graph of mesh connectivity AFTER decomposition

Particle Distribution



Particles occur in every right branch of a bifurcation

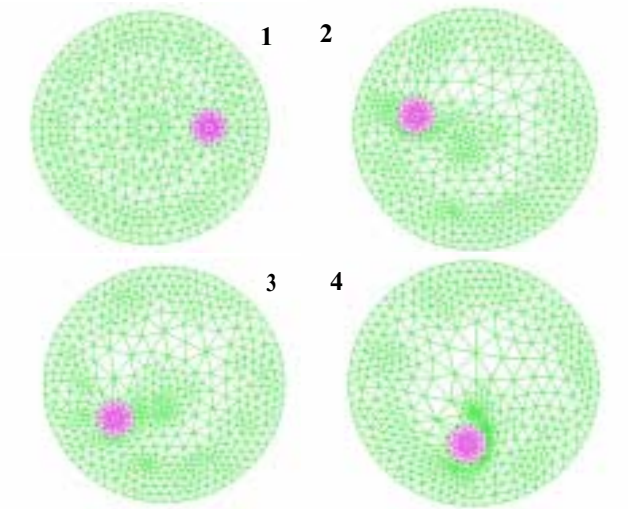
Contours of the Flow Field



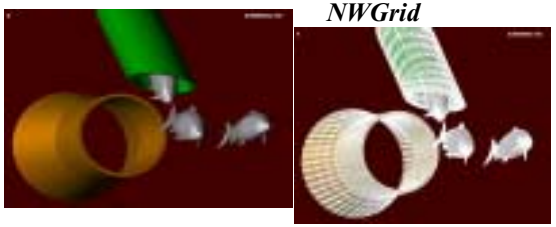
Grid generation is a fundamental part of any mesh-based computational physics problem. ***NWGrid/NWPhys*** integrates automated grid generation, time-dependent adaptivity, applied mathematics, and numerical analysis for hybrid grids on distributed parallel computing systems. This system transforms geometries into computable hybrid grids upon which computational physics problems can then be solved.

NWGrid is used as the preprocessing grid generator for ***NWPhys***, setting up the grid, applying boundary and initial conditions, and defining the run-time parameters for the ***NWPhys*** calculations. ***NWGrid*** provides the grid partitioning functions and the time-dependent grid generation functions for adaptive mesh refinement (AMR), reconnection, smoothing, and remapping. ***NWPhys*** moves the grid according to forcing functions in non-linear physics drivers and ***NWGrid*** fixes it up based on grid topology and grid quality measures. Extensions of ***NWPhys*** include incorporating new packages for fluid-solid interactions, computational electro-magnetics, particle transport, chemistry, and aerosol transport.

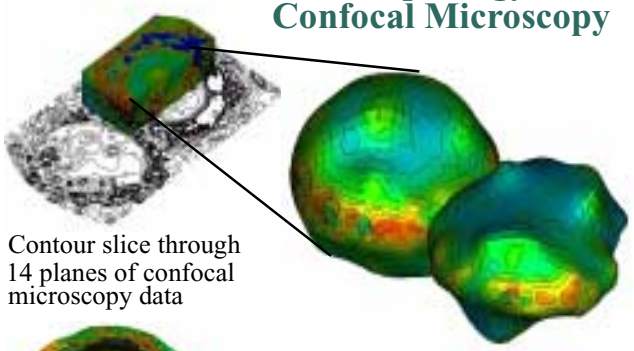
Time-Dependent Delaunay Mesh



Fish Entering Shear Layer



Cell Morphology from Confocal Microscopy



Contour slice through 14 planes of confocal microscopy data

3-D volume grid showing the reconstruction of the 2 cells with a volume distributed field mapped onto it

Shows the nucleus

Shrink Wrapping DNA Strand and Gridding it into a Matrix