Tsunami simulation using the OP2 parallel framework

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Oxford e-Research Centre

25th Biennial Conference on Numerical Analysis

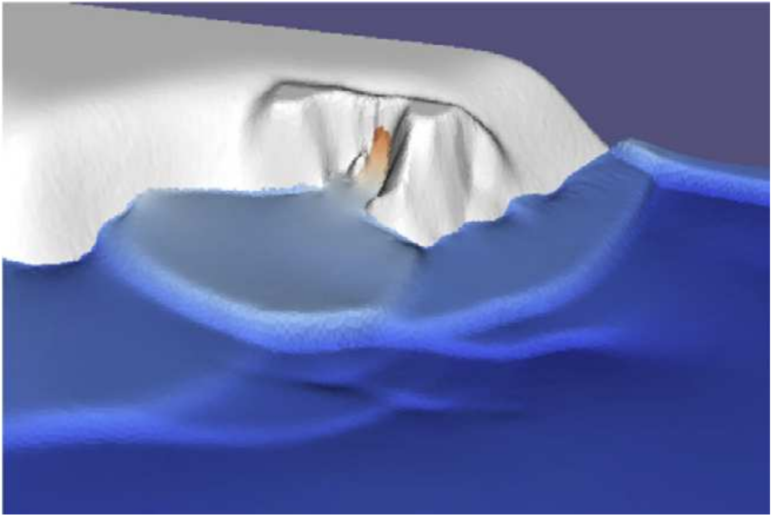
June 25th, 2013

VOLNA

- VOLNA is a Tsunami simulation code developed by Denys Dutykh, Raphaël Poncet and Frédéric Dias, and used by Serge Guillas at UCL
- modelling uses 2D shallow water equations, discretised on triangular meshes
- 3 state variables per cell:
  - water height h
  - velocity components u, v
- bathymmetry (height of sea-bed) is also stored, and modelling allows for wetting as waves run up onto dry ground
- VOLNA = wave in Russian

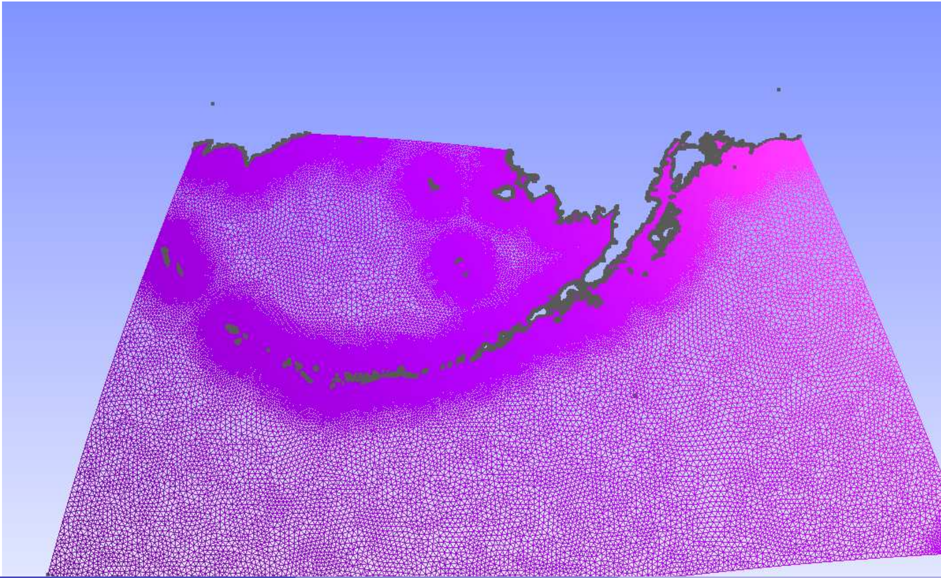
VOLNA

Tsunami simulation at Catalina Island in California



VOLNA

Grid for Alaskan Aleutian islands



VOLNA

Original code was written in C++

- strongly based on object-oriented programming (OOP)
- used STL and Boost C++ libraries
- strong emphasis on clarity of programming, and flexibility to experiment with new algorithms
- no parallel capability
- in some places OOP approach led additional data movement, with large temporary arrays being constructed
- our goal was to develop a new parallel version supporting
    - OpenMP parallelism on multicore x86 CPUs
    - CUDA parallelism on NVIDIA GPUs
    - MPI distributed memory parallelism for clusters of CPUs or GPUs
    - parallel file I/O
- total development effort – about 3 man-months using OP2

HPC Software Challenge

Problem:

- application developers want the benefits of the latest hardware but are very worried about the development effort required
- want to exploit multicore CPUs (using OpenMP) and many-core GPUs (using CUDA), and also run on clusters
- however, hardware is likely to change rapidly in next few years, and developers can't afford to keep changing their codes

Solution?

- high-level abstraction to separate the user's specification of the application from the details of the parallel implementation
- aim to achieve application level longevity together with near-optimal performance through re-targetting the back-end implementation

OP2

- open source project based on a collaboration between Oxford and Imperial College
- based on OPlus (Oxford Parallel Library for Unstructured Solvers) developed over 15 years ago for a Rolls-Royce CFD code on distributed-memory clusters
- supports application codes written in C++ or FORTRAN
- looks like a conventional library, but uses code transformation to generate CUDA for NVIDIA GPUs and OpenMP for CPUs
- keeps OPlus abstraction, but slightly modifies API

OP2 Abstraction

- sets (e.g. nodes, edges, faces)
- datasets (e.g. flow variables)
- mappings (e.g. from edges to nodes)
- parallel loops
  - operate over all members of one set
  - datasets have at most one level of indirection
  - user specifies how data is used
    (e.g. read-only, write-only, increment)

Restrictions:

- set elements can be processed in any order, doesn't affect result to machine precision
  - explicit time-marching, or multigrid with an explicit smoother is OK
  - Gauss-Seidel or ILU preconditioning is not
- static sets and mappings (no dynamic grid adaptation)

OP2 API

```
void op_init(int argc, char **argv)

op_set op_decl_set(int size, char *name)

op_map op_decl_map(op_set from, op_set to,
                   int dim, int *imap, char *name)

op_dat op_decl_dat(op_set set, int dim,
                   char *type, T *dat, char *name)

void op_decl_const(int dim, char *type, T *dat)

void op_exit()
```

OP2 API

Example of parallel loop syntax for a sparse matrix-vector product:

```
op_par_loop(res,"res", edges,
  op_arg_dat(A,-1,OP_ID, 1,"float",OP_READ),
  op_arg_dat(u, 0,col,1,"float",OP_READ),
  op_arg_dat(du,0,row,1,"float",OP_INC));
```

This is equivalent to the C code:

```
for (e=0; e<nedges; e++)
   du[row[e]] += A[e] * u[col[e]];
```

where each “edge” corresponds to a non-zero element in the matrix `A`, and `row`, `col` give the corresponding row and column indices.

OP2 API

Example of one parallel loop in VOLNA:

```
op_par_loop(SpaceDiscretization, "SpaceDisc", edges,
  op_arg_dat(data_out, 0,edgesToCells, 4,"float", OP_INC),
  op_arg_dat(data_out, 1,edgesToCells, 4,"float", OP_INC),
  op_arg_dat(edgeFluxes, -1, OP_ID, 3,"float", OP_READ),
  op_arg_dat(bathySource,-1, OP_ID, 2,"float", OP_READ),
  op_arg_dat(edgeNormals,-1, OP_ID, 2,"float", OP_READ),
  op_arg_dat(isBoundary, -1, OP_ID, 1,"int", OP_READ),
  op_arg_dat(cellVolumes,-2,edgesToCells,1,"float",OP_READ)
);
```

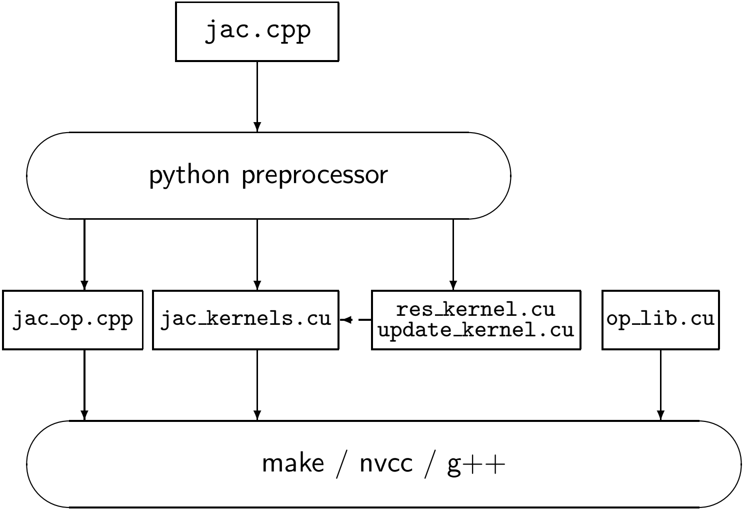
User build processes

Using the same source code, the user can build different executables for different target platforms:

- sequential single-thread CPU execution
  - no code generation – just uses a header file
  - purely for program development and debugging
- CUDA for single GPU
- OpenMP for multicore CPU systems
- MPI plus any of the above for clusters

CUDA build process

Preprocessor parses user code and generates new code:



Implementation Approach

Standard MPI distributed-memory parallelism:

- `Parmetis` or `PT-SCOTCH` for grid partitioning and local renumbering
- separate MPI process for each GPU, with each partition fitting within the GPUs global memory

GPU parallelism:

- partition sub-divided into blocks, each handled separately
- blocks sized to fit in shared memory for data reuse
- block colouring used to avoid data conflicts between blocks, and thread colouring to avoid conflicts within a block

CPU parallelism:

- similar block construction, with each handled by one OpenMP thread
- block colouring is again used to prevent data conflicts between blocks

Porting VOLNA to OP2

- a complete re-structuring of the code – almost no option for incremental transformation
- key numerical bits, such as numerical flux functions, kept as is
- overall time-marching control code largely the same as before
- still as readable as before (?)
- input/output data files converted to HDF5 for parallel file I/O
- VTK viewer developed for post-processing
- original input control file retained to minimise change for users

Porting VOLNA to OP2

One issue which came up was the need for better local renumbering

- on GPUs, original numbering led to poorly shaped blocks with lots of neighbours
  - up to 72 block colours required
  - poor cache efficiency (a lot of each cache line loaded not used)
- it also led to poor cache efficiency on CPUs
- improved renumbering reduced block colours to 6 on GPU, and reduced data transfer from main memory to the GPU/CPU

Another issue on CPUs was the need for enforcing thread affinity, to tie threads to the same core to maximise data reuse in the cache.

VOLNA performance

Test machine: 2×6-core Xeon (Westmere) + NVIDIA C2070 GPU

2 CPUs versus 1 GPU (different number of timesteps in each case)

Examples	Cells / edges	OpenMP	CUDA
Landslide (synthetic)	500k / 751k	18.4s	7.5s
Catalina (1993)	98k / 147k	1.2s	0.74s
Mentawi (2012)	140k / 211k	2.0s	1.05s
Vancouver (hypothetical)	2.4M / 3.6M	5.15s	2.1s

Hence, on big testcases, 1 GPU is equivalent to roughly 5 CPUs

VOLNA performance

VOLNA is memory bandwidth limited on both CPUs and GPUs.

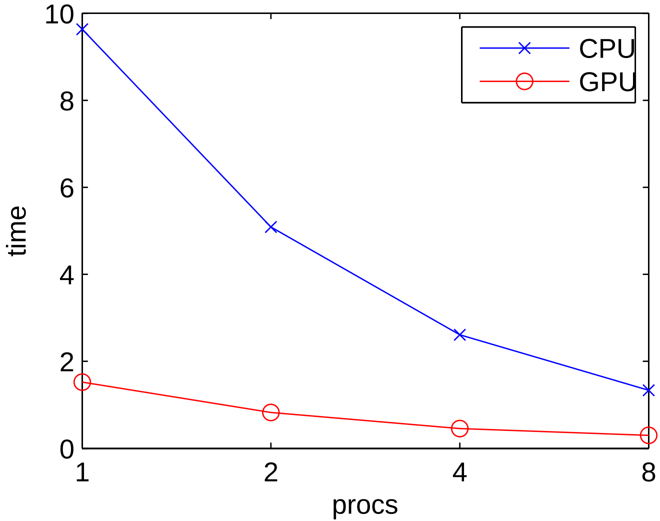
2xCPU	time	GB/s	GB/s	kernel name
	0.37	30		EvolveRK
	1.41	24	24	ComputeFluxes
	0.74	29	30	NumericalFluxes
	1.46	25	25	SpaceDiscretization

1xGPU	time	GB/s	GB/s	kernel name
	0.18	105		EvolveRK
	0.59	58	60	ComputeFluxes
	0.28	79	84	NumericalFluxes
	0.69	52	55	SpaceDiscretization

Second B/W column includes whole cache line

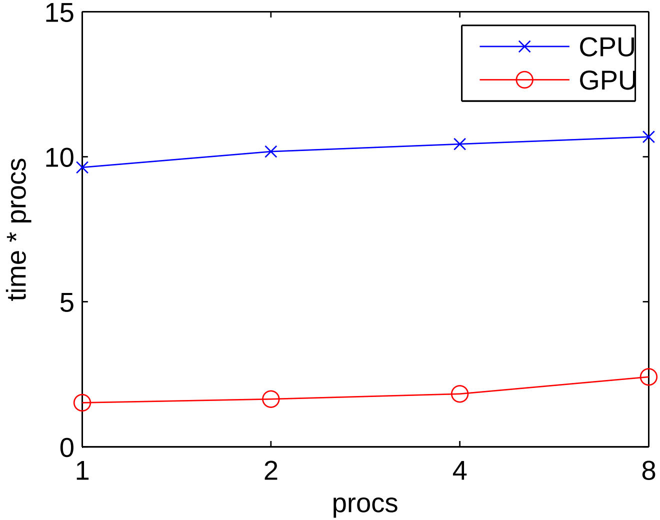
VOLNA performance

Test machine: Emerald GPU cluster with compute nodes with 6-core Intel Xeons (Westmere) + NVIDIA C2090 GPUs (Fermi)



VOLNA performance

Strong scaling is quite good on Vancouver testcase (2.4M cells)
— on other OP2 applications, weak scaling is usually better



Conclusions

- excellent scalable parallel performance has been achieved for an important tsunami simulation code
- development effort was low using OP2 framework, and code readability was maintained
- VOLNA-OP2 will now be used for new tsunami research at UCL in collaboration with Indian Institute of Science in Bangalore
- OP2 challenge is to get someone to port a major code on their own – can only really claim a tool is easy-to-use if someone else uses it!
- new EPSRC project with Bristol, Southampton and STFC will address needs of multi-block structured grid codes with a focus on two particular CFD codes

References

"The VOLNA code for the numerical modelling of tsunami waves: generation, propagation and inundation", D Dutykh, R Poncet, F Dias, *European Journal of Mechanics - B/Fluids*, 30(6):598-615, 2011

"Performance analysis and optimisation of the OP2 framework on many-core architectures", MB Giles, GR Mudalige, Z Sharif, G Markall, PHJ Kelly, *Computer Journal*, 55(2):168-180, 2012.

"OP2: an active library framework for solving unstructured mesh-based applications on multi-core and many-core architectures", GR Mudalige, I Reguly, MB Giles, C Bertolli, PHJ Kelly. *Innovative Parallel Computing conference*, 2012.

OP2 project homepage:
`http://www.oerc.ox.ac.uk/research/op2`