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Analysis of
Partial Differential Equations
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NLSEmagic

Non**L**inear **S**chrödinger **E**quation
multidimensional
Matlab-based
gPU-accelerated
integrators using
compact High-order Schemes

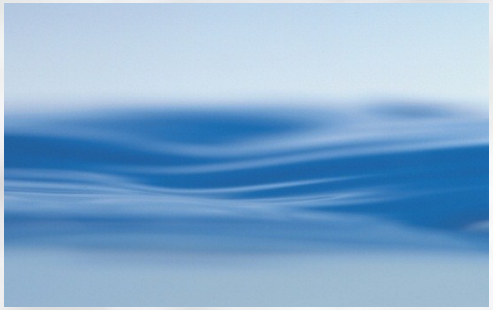
Ronald M. Caplan, Ricardo Carretero
Nonlinear Dynamical Systems Group
Computational Science Research Center
San Diego State University

Outline

- Nonlinear Schrödinger Equation
- Numerical Algorithms
- MATLAB and MEX
- GPU CUDA MEX
- Examples and Timing Results
- NLSEmagic Distribution

Nonlinear Schrödinger Equation

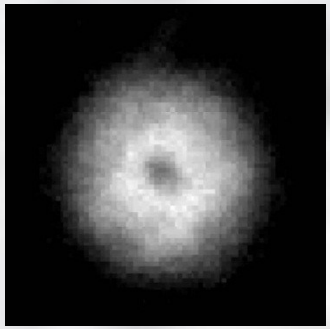
Numerous Applications



Water waves

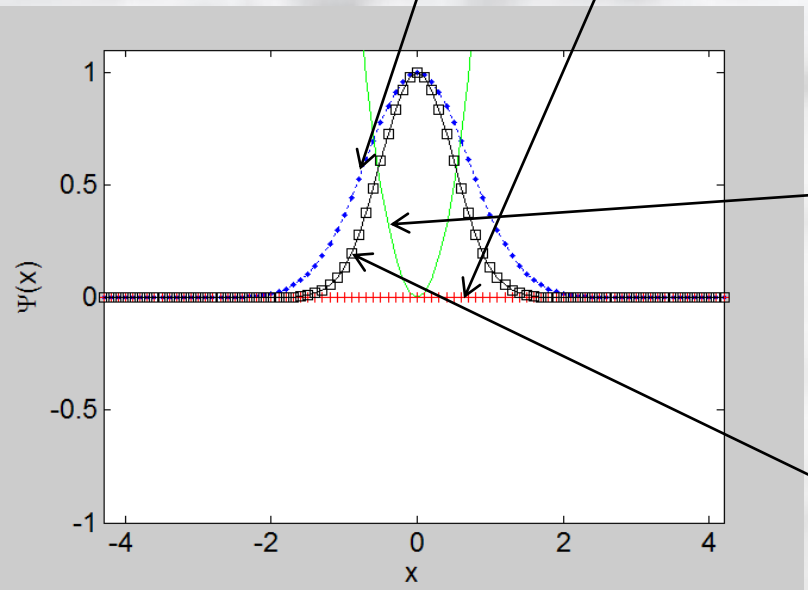
Nonlinear optics

Bose-Einstein condensates



Ψ Wavefunction – Real and Imag

$$i\,\frac{\partial \Psi}{\partial t} + a\,\nabla^2\Psi + \left(-V(\mathbf{r}) + s\,|\Psi|^2\right)\Psi = 0$$



External Potential

Parameters

Laplacian $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

$|\Psi|^2$ Observable

Numerical Algorithms

Explicit Time Finite-Difference

$$\frac{\partial \Psi_i}{\partial t} = F(\vec{\Psi})$$

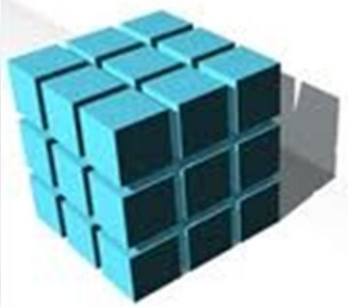
Fourth-Order Runge-Kutta (RK4)

$$\Psi^{n+1} = \Psi^n + \frac{\Delta t}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)$$

$$k_1 = F(\Psi^n) \qquad k_2 = F(\Psi^n + \frac{\Delta t}{2}k_1)$$

$$k_3 = F(\Psi^n + \frac{\Delta t}{2}k_2) \quad k_4 = F(\Psi^n + \Delta t k_3)$$

Spatial Finite-Difference



Second-Order Central Differencing (CD)

$$\nabla^2 \Psi_i = \left(\delta_x^2 + \delta_y^2 + \delta_z^2\right)\Psi_i$$

Fourth-Order Two-step High-Order Scheme (2SHOC)

$$1)\ D_i = (\delta_x^2 + \delta_y^2 + \delta_z^2)\Psi_i$$

$$2)\ \nabla^2 \Psi_i = \mathbf{A}\, D_i + \mathbf{B}\, \Psi_i$$

Boundary Conditions

Dirichlet

$$\Psi_b = B$$

$$\frac{\partial \Psi_b}{\partial t} = 0$$

Laplacian-Zero

$$\nabla^2 \Psi_b = 0$$

$$\frac{\partial \Psi_b}{\partial t} = i\left(s|\Psi_b|^2 - V_b\right)\Psi_b$$

Modulus-Squared Dirichlet

$$|\Psi_b|^2 = 0$$

$$\frac{\partial \Psi_b}{\partial t} \approx i\,\mathrm{Im}\left[\frac{1}{\Psi_{b-1}}\frac{\partial \Psi_{b-1}}{\partial t}\right]\Psi_b$$

MATLAB and MEX

MathWorks® MATLAB

- Used widely as educational tool and for research and industry
- Offers easy integrated visualizations, analysis tools. built-in math functions, easy to code, etc.

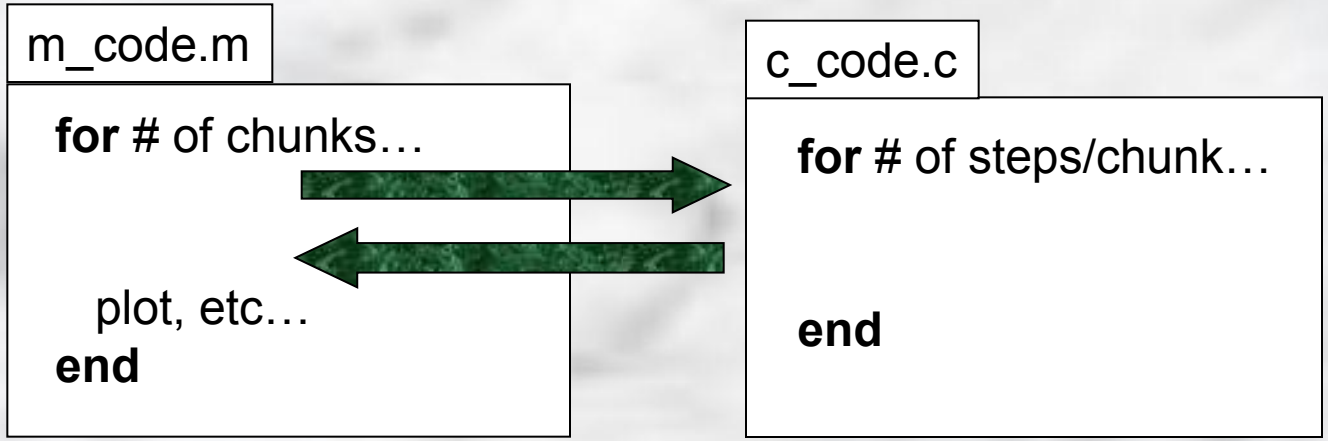
Why not use it for everything?

- Since codes are scripts (not compiled), “real” code use is SLOW

MEX

Solution

- Can write MEX files: C code with MATLAB interface.
- Easy to port if needed
- Allows compiled C code speed with the advantages of MATLAB



GPU CUDA MEX

Graphical Processing Units (GPUs)

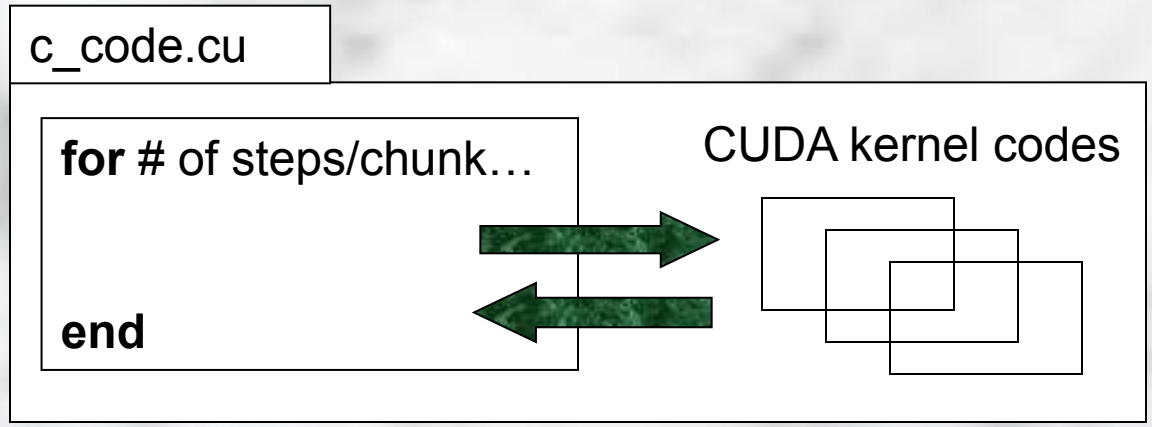
- **Cheap**: ~$1 per core for desktop card,
  ~$5 per core for compute-only workstation card.
- **Fast**: Up to **1024 cores** at ~1.5GHz
  Top card boasts peak ~ 2 **Tflops** FP, ~ 1 **Tflops** DP
- Medium-large problem capacity: RAM 1.5GB -> 6.0GB

Why doesn't everyone use it?

- **Not for all problems**
- **Learning Curve:** Need special C/FORTRAN code using CUDA API
- **Preexisting Conditions:** Translation of standard parallel code into GPU "difficult".

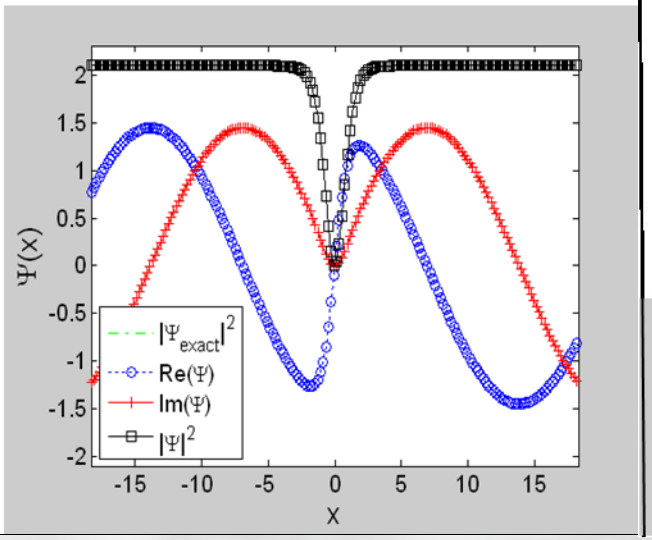
nvMEX

Set of files that allows compiling CUDA GPU codes in a MEX file

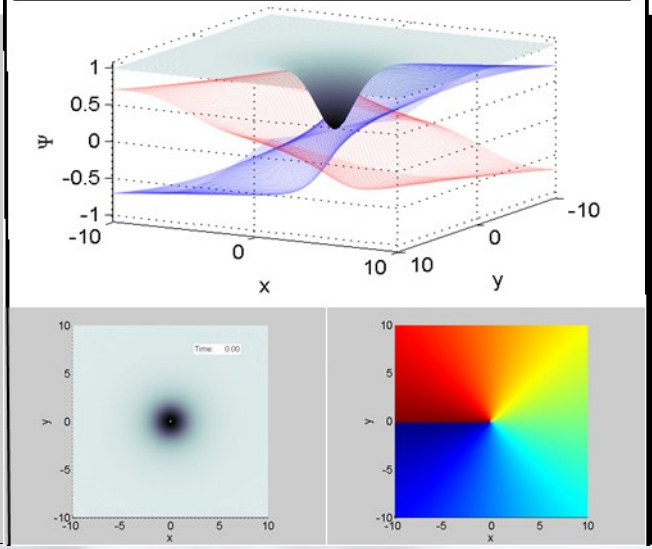


Examples and Timing Results

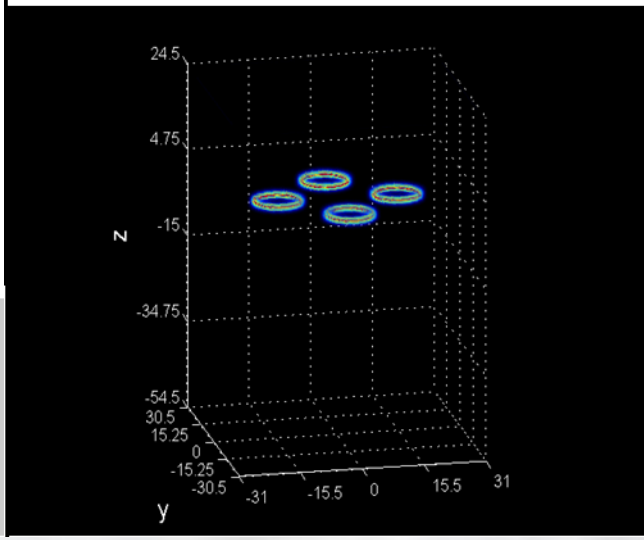
1D Co-moving Dark Soliton



2D Steady-State Vortex

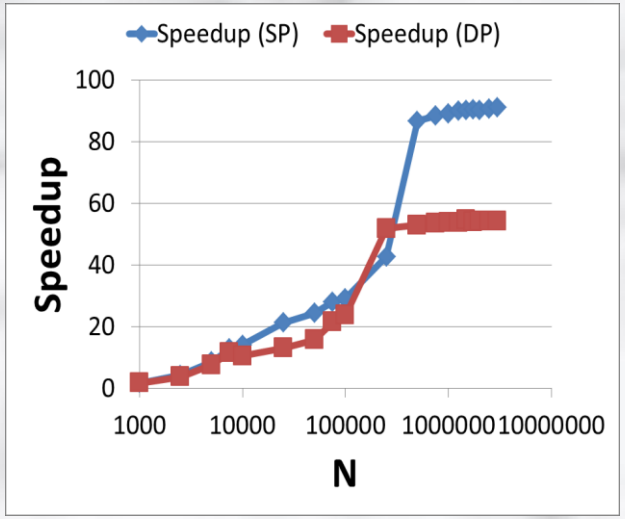


3D Dark Vortex Rings

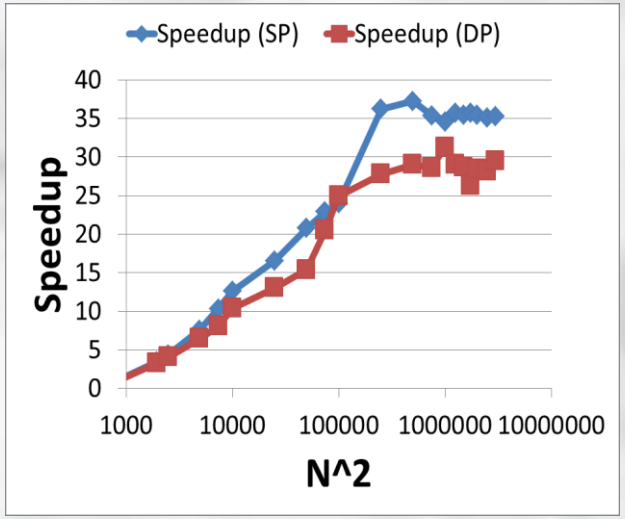


Speedup results (for similar examples):

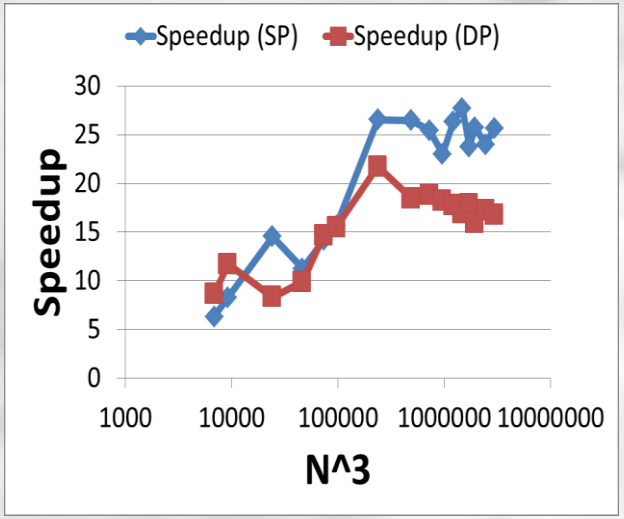
1D



2D

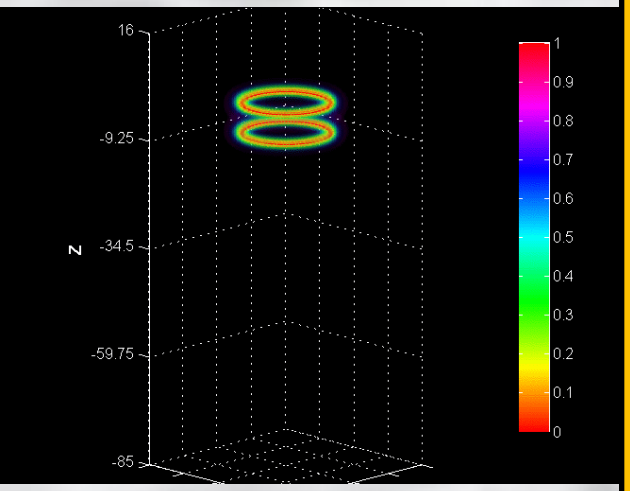


3D



Examples and Timing Results

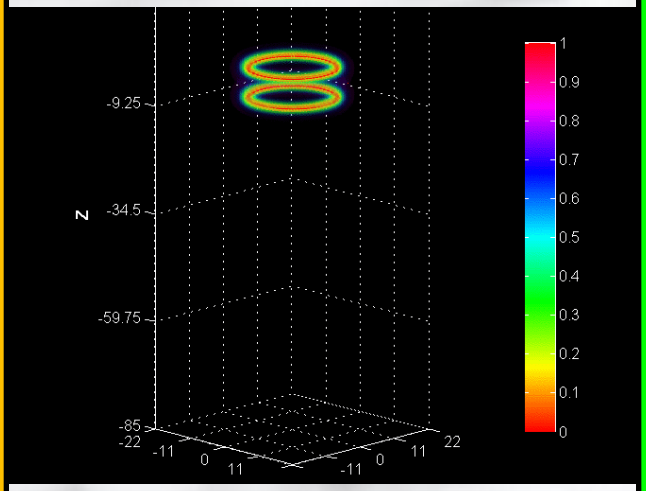
MATLAB Script



Simulation Details
Method: RK4 + 2SHOC
End time: 100.8
Time steps: 3360
k = 0.03 h = 0.5
Grid: 87x87x203 = 1,536,507
60 frames with 56 steps each
Plotting/movie time ~22.4 sec

Compute time
3:30:43

MATLAB MEX (C Code)

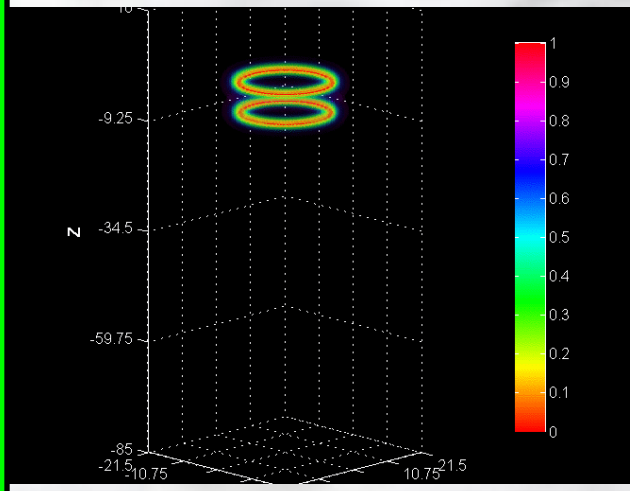


System Details
Corei3 **3.07 GHz** Dual-thread
4GB RAM 64-bit Windows 7
MATLAB R2010b **Cost~$650**

Compute time
0:37:47

Speedup
5.58X faster than script

MATLAB CUDA-MEX



GPU Details
NVIDIA GTX 580 **Cost ~$450**

Compute time
0:01:24

Speedup
26X faster than MEX

Speedup
150X faster than script!

NLSEmagic Distribution

http://www.nlsemagic.com

- Full code package available as a free download.
- Setup guide documentation.
- Full research scripts and additional documentation to come soon…

NLSEmagic

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Questions?